NBS TECHNICAL NOTE

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STATUS REPORT

National Standard Reference Data System

April 1966

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TECHNICAL NOTE 289

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April 1966

Edward L. Brady, Editor

Office of Standard Reference Data
National Bureau of Standards
Institute for Basic Standards
Washington, D.C., 20234

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FOREWORD

In June 1963, the technical agencies of the Federal Government, acting through the Federal Council for Science and Technology and the President's Office of Science and Technology, established the National Standard Reference Data System. The objective of the NSRDS is to provide compilations of critically evaluated property data to the technical community of the United States, under central coordination to minimize duplication and to assure timely coverage of the nation's needs. Responsibility for the administration of the system was assigned to the National Bureau of Standards, which established the Office of Standard Reference Data for the purpose.

The present report summarizes primarily the status of the activities of the NBS Office of Standard Reference Data and the data compilation projects with which it has established a working relationship. Emphasis is placed on the activities which NBS-OSRD has funded, in order that the reader may see the way in which NBS has made use of its resources. In addition, an effort has been made to avoid giving the impression of claiming credit for activities that NBS-OSRD has had little to do with. For these reasons, it may seem that some important projects have received only passing mention in the report. The amount of detail given for any project should not be taken as an indication of judgment on its importance.

The entire professional staff of the Office of Standard Reference Data has participated in the writing of this report. Consequently, there are inevitable inconsistencies of style and format.

The staff of OSRD would greatly appreciate receiving any comments that the readers of the report would care to make. Since the function of the Office is to provide a service to the technical community, any views on ways to improve the service are welcome. The response and reaction of potential users is essential if the system is to be effective.

Edward L. Brady

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A B S T R A C T

This report summarizes the status of the activities of the NBS Office of Standard Reference Data as of March, 1966. It provides a detailed review of the data compilation activities within the seven broad categories within the technical scope of the program: (1) nuclear data, (2) atomic data and molecular data, (3) solid state data, (4) thermodynamic and transport data, (5) chemical kinetics, (6) colloid and surface properties, and (7) mechanical properties. Plans for an information services program are also outlined. Certain problem areas are identified. The appendix includes a listing of properties with which the program is concerned and a listing of the advisory panels of the Office of Standard Reference Data.

Key Words: nuclear data, atomic and molecular data, solid state data; thermodynamic and transport properties, chemical kinetics, colloid and surface properties, mechanical properties; information services, standard reference data

THE NATIONAL STANDARD REFERENCE DATA SYSTEM

STATUS REPORT - October 1965

I. GENERAL SURVEY

A. Origin of National Standard Reference Data System

In June 1963, the Director of the Office of Science and Technology, acting in his capacity as coordinator of the technical activities of the federal government, promulgated a federal policy establishing the National Standard Reference Data System, in order to provide on a national basis critically evaluated data in the physical sciences. According to the statement of the Director of OST, "the intent is to provide an articulated system of activities under such coordination and direction as to ensure a compilation of data meeting quality standards, and also to maintain continuous policy guidance of the system at the level of the Executive Office." This action was taken upon the recommendation of the Federal Council for Science and Technology, which recognized that many government agencies, without coordination or central guidance, had been sponsoring activities of the type to be encompassed within the National Standard Reference Data System. To avoid duplication and at the same time to assure adequate and timely technical coverage, the Federal Council for Science and Technology decided that additional measures needed to be taken; the National Standard Reference Data System was the result.

In view of the National Bureau of Standards' responsibility for broad leadership of the national measurement system, which includes not only the standards for making measurements but also the results of those measurements which can be considered to be of lasting value, the Federal Council recommended that the National Bureau of Standards be given responsibility for administration of the National Standard Reference Data System. The directive given by the Director of the Office of Science and Technology calls upon NBS to promote the basic objective of providing standard reference data to the technical community; to coordinate standard reference data activities of DoD, AEC, NASA, NSF, Commerce, Interior, and other government agencies; to operate a national standard reference data center at NBS; to establish standards of quality for various products of the NSRDS; and to establish standards of methodology and such other functions as are required to ensure the compatability of all units of the NSRDS.

B. NBS Office of Standard Reference Data

In order to fulfill his responsibilities to the National Standard Reference Data System, the Director of the National Bureau of Standards has established an Office of Standard Reference Data (OSRD) within the NBS Institute for Basic Standards. This office has been assigned coordination and contracting responsibility for the conduct of the NBS role

in the NSRDS, but this office has no direct operational responsibility for the data centers, within and outside NBS that constitute the NSRDS. The present report contains a brief review of the actions taken and progress made by the Office of Standard Reference Data since its establishment together with brief descriptions of the important systematic, continuing data compilation projects considered to comprise the major part of the National Standard Reference Data System.

C. General Plan of Operation

The basic philosophy behind the plan of operation of the National Standard Reference Data System is that the program is a cooperative endeavor of the entire technical community of the United States. Its premise is that preparation of compilations of critically evaluated property data is of vital interest to nearly every technical man in the practice of his profession, and the needs and wishes of these men are to be determining factors in the guidance of the System. All technical agencies of the government have found it necessary to sponsor data compilation activities of the type appropriate to the NSRDS in order to fulfill the requirements of their missions; these activities, by virtue of their very existence, are part of the total complex making up the National Standard Reference Data System.

In this total complex the National Bureau of Standards has assumed a special role, in accordance with the directive from the Office of Science and Technology, but the NBS makes no proprietary claims to ownership of the NSRDS and endeavors at all times to maintain two-way channels of communication with persons involved with the development of the program in all agencies, both governmental and non-governmental.

As stipulated in the OST directive, the technical scope of the National Standard Reference Data System is physical science. For management purposes within NBS-OSRD, the scope has been divided into seven broad categories: (1) nuclear data, (2) atomic and molecular data, (3) solid state data, (4) thermodynamics and transport data, (5) chemical kinetics, (6) colloid and surface properties, and (7) mechanical properties. In each of these categories an effort has been made to identify properties of interest, survey existing activities, establish priorities for expansion of existing projects and for initiation of new ones, and to enter into contractual or other financial arrangements with individuals or groups who are both competent and interested in doing the required work. In all of these tasks, the NBS-OSRD has relied heavily upon consultation with panels of specialists in the fields of data. Some of these panels are comprised of existing or slightly modified committees of the National Academy of Sciences, while others have been specially assembled for the special needs of the OSRD program. The memberships of these panels are listed in Appendix A. Of great aid in the development of the program has been the Office of Critical Tables of the National Academy of Sciences-National Research Council which has proved to be a mine of information about existing data compilation activities in all parts of the world and has greatly assisted the NBS Office of Standard Reference Data in communicating with the technical community.

In addition to developing a comprehensive set of data compilation activities covering the desired scope of physical science, the NBS Office of Standard Reference Data has the responsibility for ensuring

that all products of the National Standard Reference Data System are made conveniently accessible to data users in the technical community. This requires OSRD to develop mechanisms for letting the users know what is available, for publication and distribution of the products (if not otherwise disseminated), and for providing special user services employing the resources of the central collection of compilations in OSRD.

Upon the recommendation of the advisory panels, the NBS-OSRD has concentrated its efforts and financial resources on filling gaps in coverage and expanding the level of effort in existing projects, leaving for future emphasis the development of the contemplated information services. In initiating new data compilation projects, the OSRD has attempted in all cases to establish these as an adjunct of the program of an active experimental group in the field of the data, in accordance with the recommendation on such activities made by the "Weinberg Report." In general, the OSRD takes every opportunity to promote the view that data evaluation and compilation are a normal aspect of a professional career and should be accorded the same respect, dignity, and pay as other scientific professional activities.

D. Overview of Status of OSRD Activities

Within the philosophy and general plan of operation just previously outlined, significant progress has been made in coordinating and extending existing coverage in the technical categories, especially in the areas of thermodynamics and transport properties and in atomic and molecular properties. These two categories have been judged to be of highest priority for additional effort. In the field of nuclear data, existing activities sponsored by the U.S. Atomic Energy Commission provide nearly adequate coverage of the technical scope required, although the level of effort needs to be increased to meet the rapid rate of appearance of new data. In the category of solid state properties, existing projects provide good coverage of the more classical areas, such as structural data, but greatly increased effort on the newer kinds of data (energy levels, band structure, interaction with radiations) has been recommended by the advisory panel. In the category of chemical kinetics, the advisory panel agreed that it was not convinced that any data in the literature were worthy of a systematic evaluation and compilation effort, and therefore, the first stage of the OSRD program should be the preparation of a series of critical reviews of the state of quantitative knowledge in certain selected aspects of the field. In the field of colloid and surface properties, the OSRD has established a cooperative relationship with the NAS-NRC Committee on Colloid and Surface Chemistry, which had been planning an extensive program of data evaluation prior to the establishment of the NSRDS. In the field of mechanical properties, there has been a preliminary critical survey by a group of NBS staff members. Its objectives are to assess whether there exists any significant body of data in this field satisfying the basic requirements of "Standard Reference Data": (1) that the material be well defined in composition and structure and (2) that the measured value be representative

of an intrinsic property of the material and not the result of an interaction between the measuring system and the material (as for example, hardness or breaking strength). The conclusion of this preliminary survey was that there probably are very few data entirely appropriate and therefore little effort has been expended on this category. However, this conclusion is regarded as tentative and is to be re-examined by a panel of specialists gathered from the academic, industrial, and governmental segments of the technical community.

The information services, as presently planned, consist of four main components: (1) a data file, with a complete collection of evaluated data compilations, indexed and stored for rapid retrieval, (2) an inquiry service to provide replies to questions relating to property data and to prepare a current awareness service, (3) a compilation production service, to provide assistance in planning the information and data flow from the original source in the literature through the evaluation process at a data center and on to the user, and (4) an analysis and user relations service for providing intelligence and feedback on the systems' users needs.

The data compilation projects in the various categories and the information services operation are described in more detail in the following sections of this report.

E. Problems

1. Quality Standards

The directive from OST calls upon NBS to take the lead in establishing standards of quality for the products of the NSRDS. Considerable thought has been given to this matter without, as yet, having produced a practical solution.

In general, basic criteria on which everyone agrees are that the data shall be evaluated by a specialist of mature judgment in the field of the data and that all publications shall have adequate documentation on the sources of the data so that the user may, if he wishes, carry out his own evaluation.

From this point on, however, opinions diverge. For example, what does "critical evaluation" mean? In past practice in some data centers, it means that the experimental technique has been reviewed, calculations have been at least spot-checked, values of the fundamental constants checked to be sure latest values were used, temperature scale checked, if appropriate, and limits of experimental uncertainty independently assessed. In other centers, the data evaluator has decided, for intangible reasons which he has difficulty formulating, that one particular value in the literature was "better" than another value. (Such a judgment by a specialist of broad experience should not be under-rated; the value obtained is much more likely to be accurate than the value obtained by unweighted averaging.) Most people agree that the first procedure provides a better "critical evaluation" than the second. However, for many practical purposes such review is not justified and the second procedure, or an intermediate one, is employed.

The question immediately arises, then, as to what degree of critical evaluation is required in order that a compilation should be considered "Standard Reference Data." This question is still unresolved, though in a few cases efforts are being made to devise sets of standards for experimental conditions in order for the results to be considered for inclusion in a compilation of standard reference data.

A related question arises from the observation that two equally competent specialists considering the same set of data may produce different evaluated results. There will be so many such instances that it will not be practical to insist that the persons involved get together and agree on a value, nor would the benefit of reaching agreement justify the cost in time and money. Should one of the values be chosen as the "reference," should both, or neither? At the present time, the staff of the Office of Standard Reference Data favors indicating both sets of data as "SRD" but further consultation and discussion is required before the matter is resolved.

2. Communications With Data Users

Surveys made by many groups, as well as by the NBS Office of Standard Reference Data, show clearly that the great majority of technical men is quite ignorant of the information and data resources available. It is essential for the NBS-OSRD and the various components of the NSRDS to establish effective, continuing communication with the users and potential users of the products of the system. The experience of existing data centers indicates that normally several years are required to establish reasonably good communication, and, even with well known centers, there is no way to determine how many potential users are unaware of the existence of the center and its products. The Office of Standard Reference Data is seeking ways of rapidly improving the two-way flow of information between itself and the members of the technical community.

3. Communication and Work-Sharing Among Related Data Centers

Some data centers now in existence produce results used by other centers as input data in their computations or as a means of checking consistency of their data. In other cases, data centers may cover much of the same literature in their search for relevant data in their own areas of competence. In the interest of economy and efficiency it is, of course, highly desirable for the groups involved to maintain frequent contact with each other and to the maximum extent, share the tasks common to each. The staff of the Office of Standard Reference Data works with the responsible operating officers in such cases to develop more efficient working arrangements, but much remains to be done.

II. PLANS FOR INFORMATION SERVICES

During the past year we have spent considerable effort on developing plans for the handling of information in the National Standard Reference Data System. These plans are concerned with the information with which the System deals; with the logical organization of this information, its acquisition and physical storage; with methods of locating desired information items in storage; and with retrieving and displaying or communicating them. The present section summarizes the major conclusions which have been reached in this effort.

It is expected that the information system of NSRDS will undergo evolutionary changes for a number of years. Many of these cannot be clearly foreseen as yet. Despite this uncertainty, two basic policy decisions have been adopted:

1. Ultimately, the NSRDS information system will involve the use of large electronic digital computers in a crucial way (though not necessarily to the complete exclusion of manual methods).

2. For the present, the system will operate only with conventional and, in the main, manually operated files.

We visualize the transition from System 2 to System 1 as taking place gradually rather than all at once. We plan to avoid the introduction of intermediate systems not compatible with the final large scale system. We base our planning on the assumption that the bulk of such a system can be implemented in 3 to 5 years. We do not anticipate that mechanization will ever be carried to the extreme of complete exclusion of all human functions. Rather, we envisage a system of man-machine cooperation.

The Office of Standard Reference Data operates an information service at NBS. This information Services Operation (ISO) is expected to consist of four units, concerned with (1) compilation-production services, (2) inquiry services, (3) the data file operation and analysis, which supports the other two units, and (4) analysis and user relations services.

A. Compilation-Production Services

Compilation-production services include the dissemination of information, either periodically or occasionally, on our own initiative. Some of this is now being done by technical data centers, and will continue to be handled by them, with or without assistance from OSRD. ISO will not duplicate any of these efforts but will attempt to supplement them by publications covering the field of reference data in general, or cutting across the lines of several data centers, or falling between them.

The activities of the compilation production unit will be concerned with periodical and aperiodical publications.

A periodical news or current awareness service, concerned with events in the field of data on properties of materials, is contemplated. New data compilations which have been published, projects undertaken or completed, contracts awarded, new mechanization techniques, etc. would be listed.

Among aperiodic publicational activities, there is first of all the "National Standard Reference Data Series" of the National Bureau of Standards published by the Government Printing Office, of which several numbers have al-

ready appeared. The series will contain tables of data compiled and evaluated under the auspices of OSRD and related material. It is intended to supplement, rather than supplant, the publication activities of technical data centers and other interested organizations. Thus the NSRD Series will have for primary subjects those compilations produced at NBS, or by organizations which for some reason or other cannot undertake publications, or those for which there is no appropriate technical data center, as well as state-of-art reports, lists of compilations considered to be standard reference data, reports on classification, indexing, mechanization, and other topics of interest to data compilers, evaluators, and users in general.

In addition to publishing the NSRD Series, OSRD will produce data in loose-leaf form, machine readable media such as tapes or punched cards, or other formats which prove to be widely useful.

The nature of much of the material to be published by NSRDS is such that it is likely to benefit from recent developments in computer-controlled typesetting. One reason for this is that much of the material in tables of physical data originates as computer output, and is therefore easy to record on machine readable media. Another reason is the facility for rearranging, updating or otherwise revising the material. An example is the volume "Crystal Data Tables" now being prepared for publication by photocomposition. The original information is being keypunched in essentially the same format in which it is to appear in print, and this part of the operation offers no great advantage over manual typesetting. But from the keypunched information it will be possible to produce alphabetical indexes for authors, names and formulas of chemical compounds, all by automatic sorting, checking and editing. In subsequent editions, only the new or revised material will have to be newly keypunched, the computer will insert it in the proper place, change pagination as needed, update the indexes.

There are several steps which OSRD has taken or plans to take in the near future in order to assist in the transition to mechanized publication. The first of these is the acquisition of a Mergenthaler linofilm keyboard, which produces the 15-hole punched paper tape needed to drive the linofilm composition machine. One of the advantages of having this device at NBS is that keypunching can now be done under the direct supervision of the scientists responsible for the preparation of a manuscript. Another step in the same direction is the procurement of a modified tape typewriter (Smith-Corona-Marchant) which will accept a number of special character inserts (similar to the commercially available "Typits") and at the same time produce a punched paper tape. Because of its lower cost, this tape typewriter is preferred for material of simple typography. Finally, an IBM Document Writer has been acquired by one of the data centers located at NBS and is being used with great success for material of intermediate typographical quality.

These recording methods can be aided by performing some editing functions on a computer. Several computer codes for such purposes have been written; so far, each of these codes was tailored to one particular publication. One of the efforts in which OSRD expects to engage in the near future is the production of more generally applicable computer codes for publication editing.

B. Inquiry Services

Inquiry services may result in four kinds of action taken in response to requests for information: (1) Referral (2) Reference (3) Documentation (4) Data Information. Referral means that the question is referred to another organization or individuals. By reference is meant a listing of relevant literature. Documentation goes one step further and includes furnishing of micro-stored or hard copies of the referenced literature. Data Information implies furnishing not only a listing of the requested data, but also any necessary explanation, caution, etc.

Circumstances suggest strongly that inquiry-answering services to scientists and engineers should begin at once, without delay. Not only should the benefits accruing to the technical community from the availability of such services not be postponed by several years pending the creation of data files and systems, but the creation of the systems will itself be aided by the experience which OSRD will acquire in the process of rendering services.

It follows that, in many fields, requests for data will have to be answered before standard reference data have been so designated. In such cases, rather than merely indicating to the inquirer that no SRD are as yet available, it will be preferable to give him whatever information can be found in the literature or through personal inquiries. A suitable disclaimer will be appended to such replies, cautioning the user that the information has not been evaluated by NSRDS.

In the early years, while NSRDS is still developing, a large portion of technical inquiries received is likely to be referred to experts. Furthermore, until OSRD has accumulated some experience it will be well to have all technical answers, even those routinely prepared by OSRD from its own files, checked by a specialist. The experts to whom questions are referred can be taken from the following groups: (1) technical area managers of OSRD (2) data centers which adhere to OSRD (3) divisions at NBS outside the OSRD, and (4) other scientists. ISO should furnish references to the literature and/or copies of pertinent documents only if this can be done without undue effort.

As time goes on and mechanization of the system progresses, an increasing number of inquiries will be answered by reference to the computer-stored data file.

C. Data File

The data file unit, the only one activated so far, has been engaged in organizing its activity. One of its first tasks is to acquire some information on the need for its services and the tools available for rendering them.

A major bibliographic survey of existing compilations of quantitative data on physical and chemical properties of materials is being undertaken. It is expected that this survey will cover all existing compilations of data, whether published in the open literature or in report form; as far as possible it will also include unpublished manuscript compilations. The survey will not have to start entirely from scratch. The Office of Critical Tables of the NAS-NRC has collected a list of some of the best known data compilations, and is continuing this work on a small scale. OSRD has on its own assembled a modest collection

of compilations. These two collections could be used as starting points. There also exist surveys in some specialized fields; for instance, the Nuclear Data Project at Oak Ridge has made a survey of compilations of nuclear data; it is not yet complete, but the work is being continued.

The most important preparation for the operation of ISO is the organization of information. OSRD has sponsored two pilot studies of classification. One of these proceeded empirically in line with modern trends in documentation; the other took a fundamental approach of basing the classification on the underlying properties of matter. Both are long-range efforts. For immediate use OSRD has designed a system of classifying physical properties of materials, following the lines of conventional hierarchical classification. It consists of a few hundred classes, which have proved to be amply adequate for classifying the present library of ISO and will undoubtedly be adequate for any foreseeable expansion of it.

D. Analysis and User Relations

A data system's reason for existence is the use to which it is put. Therefore, the user is the most important element in the data cycle chain. The analysis and user relations unit has the task of understanding the requirements both present and future of the NSRDS' actual and potential users; the unit has the responsibility for providing the Services with information on how best to meet these needs. This activity will have another important task - developing feedback mechanisms to evaluate the services provided.

E. Long Range Mechanization Problems

Up to this point we have dealt with the short range problem of operating an information system based on conventional files and library collections. We now turn to the longer range problem of mechanization.

It is probable that OSRD will use the general purpose, large computer of NBS. Provision will have to be made for certain peculiarities of the OSRD operation.

(1) The amount of data to be stored for OSRD is so great that it is impractical to keep them on cards or tape and read them into the computer for each run anew. In this respect OSRD is, and probably will remain, unique among NBS computer users. It will be necessary to acquire a separate storage component, which would be purchased or rented by OSRD and reserved for its exclusive use, and which would be connected to the computer main frame. Suitable storage devices are now available from several manufacturers.

(2) It will be desirable to have facilities for remote on-line access to the central computer. A console should be located in the OSRD offices from which a user can contact the central computer, wait for the end of the current problem (or in the case of a long problem, interrupt it), read into the computer a small amount of instructions and data, have the instructions executed and immediately see a small volume of results. Large-volume output would remain on tape in the computer room and be available to the user there.

(3) At a later time it may also be desirable to use similar remote stations in distant cities. One of the tasks which the system will have to face is to supply information to users anywhere in the country. Although mail or telephone can be used for this purpose, a great deal more could be accomplished if users could be given direct access to the computer file. There are in principle two ways in which this can be done. One can enable laboratories throughout the country to obtain on-line connection, via long-distance telephone lines, to the central computer and information store at OSRD; or one can duplicate this store in numerous geographically dispersed computing facilities. There is no point in drawing up a precise balance sheet of costs at this time, since the information file does not yet exist, will take several years to compile, and some cost items may change radically in the meantime. In any case, we envisage the establishment of a nationwide network, either of secondary centers or of telephone access to the primary center, as something to be done only after the primary center itself has been in operation for awhile.

Experiments in remote on-line operation have been carried out successfully. This mode of operation involving man-machine interaction is expected to be of importance in cases where a question is at first not precisely formulated, and is successively sharpened on the basis of replies from the computer. Past experience of libraries and other information centers indicates that this is a typical and frequent situation.

III. NUCLEAR DATA PROJECTS

In the field of Nuclear Science, compilation activities have been undertaken almost from the beginning of large scale efforts dating back twenty-five years. A single cognizant governmental agency, the Atomic Energy Commission, has existed in this area, and has sponsored appropriate compilations. It is perhaps, for this reason, that data compilation coverage is more complete probably than in most other physical science fields. Recently Academic Press has undertaken the publication of a Journal of Nuclear Data, which will concentrate entirely on the publication of compilations of data in the nuclear field. This journal is edited by Dr. Katherine Way of ORNL.

Below is a brief survey of nuclear data compilation activities presently being undertaken. There is no special significance to the order of the listing. The list comprises compilation centers or small groups where a form of continuous compilation activity is being undertaken. In addition to the centers listed here there are a large number of individual compilations which are being undertaken to serve a specific need or purpose.

I. Compilations in the United States

A. Nuclear Data Group at Oak Ridge National Laboratory headed by Katherine Way. The main product of this group is the familiar nuclear data sheets. The nuclear sheets contain all the information known about nuclei from A=21 through A=212. In the future the product will appear in the Journal of Nuclear Data.

B. Charged Particle Cross Sections. This center is also located at Oak Ridge National Laboratory and is headed by Francis McGowan. The title is self-explanatory of the work of this group. Cross sections for various medium weight nuclei have been published. The remainder of the nuclei will be published in the nuclear data journal previously mentioned.

C. Sigma Center. This center is responsible for neutron cross sections for all energies and covering all nuclei. The group is headed by Murray Goldberg and its product is the familiar Barn Books BNL-325 and BNL-400.

D. The Neutron Cross Section Center at Lawrence Radiation Laboratory at Livermore, headed by Robert J. Howerton. The product of this group is cross-section data similar to that of the Sigma Center.

E. The Reactor Physics Constants Center at Argonne National Laboratory, headed by Robert Avery. This center supplies values of those physical quantities which are of direct need in reactor physics calculations. The product has taken the form of two editions of a collection of reviews entitled Reactor Physics (ANL-5800) and an assortment of news letters.

F. Table of Isotopes. This is a continuation of a series started at the Lawrence Radiation Laboratory at Berkeley with J. M. Hollander, I. Perlman, and G. T. Seaborg as prime contributors to previous editions, which were published as issues of Reviews of Modern Physics. The sixth edition is under preparation now. The information contained here is similar to that available in the nuclear data sheets, but on a somehwat abbreviated scale.

G. Energy Levels of Light Nuclei. A new edition is now being prepared by F.Ajzenberg-Selove, and T. Lauritsen. This effort performs the same task of compilation for nuclei with atomic weights (20)that the nuclear data sheets do for heavier nuclei.

H. Chart of the Nuclides. This is the familiar wall chart of the radioactive properties of the nuclides which for the past several years has been published at Knolls Atomic Power Laboratory of the General Electric Company under the authorship of D. T. Goldman.

I. Photo Nuclear Compilation Center at the National Bureau of Standards, headed by Everett Fuller. This effort will provide bibliographic information and cross section results for gamma rays incident upon all nuclei. The Center is supported by OSRD and details of its operation are provided in the last section of this report.

II. Compilation Centers in Europe and Asia

A. The European Neutron and Data Compilation Center at Saclay, France. This is a data compilation center being set up to maintain up-to-date indices of bibliographic references to all neutron experiments and will presumably perform the same function in Europe that the Brookhaven Center performs in the United States. In addition, data evaluation will be undertaken.

B. The Central Bureau of Nuclear Measurements at Geel, Belgium, has sponsored the compilation of certain neutron reactions such as np, n , and n, 2n. A report has been published by H. Lisskien and A. Paulsen, with this compilation. In addition, other compilations will be undertaken.

C. A similar sort of operation to that described above is performed in Sweden under the sponsorship of A. B. Atomenergi and the Research Institute of National Defense. Reports such as Cross Sections for Neutron Inelastic Scattering and n, 2n Processes, A Review of Available Experimental and Theoretical Data, by M. Leimdorfer, et al, and the Optical Model of the Nucleus, an Index and Abstracted Literature Review, by L. Wallin, et al, have been published.

D. The Atomic Weapons Research Establishment at Aldermaston, England, has a neutron data evaluation group headed by K. Parker. A large library of evaluated neutron cross sections is available on punched cards or magnetic tape. The computerization of this library has been undertaken, with joint association between the Aldermaston group and groups at Livermore and Los Alamos in this country.

E. Karlsruhe, West Germany. A report, Neutron Cross Sections for Fast Reactor Materials, which is very similar for the elements covered to the Barn Book published by Brookhaven, has been published and is available in report form. These neutron cross sections were compiled by J. J. Schmidt.

F. The Japanese Nuclear Data Committee. This committee was set up under Teruo Momota to compile and evaluate nuclear data of interest to reactor physics and technology. As of yet, no product or report from this committee has appeared.

G. Utrecht, Netherlands. Professor P. Endt and associates for several years have been compiling and publishing information on the energy levels of light nuclei for Z=11 to Z=20. This work includes the same information as the compilation listed in 2C above, but for somewhat heavier nuclei.

H. Mainz-Amsterdam. J. Mattauch of the Max Planck Institute for Chemistry in Mainz and A. Wapstra of Amsterdam have, for several years, issued a list of atomic masses prepared by a detailed evaluation of the available experimental data for a variety of nuclear reactions in addition to direct mass spectrometric measurements. In addition, Dr. Wapstra has prepared energy levels of very heavy nuclei, that is, for nuclei heavier than those presently treated in the nuclear data sheets.

I. International Atomic Energy Agency. Some effort is being undertaken by this agency to organize a world-wide cooperative nuclear data exchange with emphasis on neutron cross-section data.

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The Advisory Panel meeting on October 8, 1965, was provided with a summary and listing of data compilation centers in this country and throughout the world. The general conclusion of the Advisory Panel was that though the scope of effort being undertaken in nuclear data compilations was satisfactory, with certain exceptions, the intensity of effort should be increased considerable.

The Advisory Panel arrived at several working conclusions:

1. Present compilations cover, in principle, the general field of nuclear data. Exceptions, however, to this statement are in the categories of elementary particle compilation, including very high energy (GEV particle interactions); medium energy interactions (20 MEV-1000 MEV), an energy region in which the advent of higher current particle accelerators will provide a great deal more data; nuclear data of direct application to reactor technology, such as transport properties of media without reference to a particular reactor configuration; and primary cosmic radiations.

2. The number of data compilation centers, accordingly, could be increased.

3. The transmission of the most up-to-date information available to interested scientists must be improved.

4. Efforts at increasing the staffs of presently operating data centers should be encouraged.

5. The OSRD could offer a major contribution to nuclear data centers by helping them in the development of techniques for the automatic (computer) storage and retrieval of compiled data.

The Office of Standard Reference Data plans to formulate a program based on the conclusions and recommendations of the Advisory Panel.

Within NBS, the only active nuclear data compilation now going on is that within the Radiation Physics Division, under the direction of Everett Fuller, to compile data on photonuclear interactions. A description of its activity follows.

Title of Project: Compilation and Evaluation of Photonuclear Data

Principal Investigator: E. G. Fuller, Photonuclear Physics Section, Radiation Physics Division, NBS

Technical Scope and Plan of Operation: The first objective of the project is to review the literature on photonuclear reactions. Experimental results are abstracted and analyzed to evaluate the accuracy and limitations of the results. The second objective is to produce a quantitative bibliography of the literature searched. This bibliography will contain several pieces of information which define the scope of the experiment (e.g., type of reaction, method used, energy range covered). The third objective is to perform a critical evaluation of the photonuclear data in order to produce and publish a set of "best values" for photonuclear cross sections and related quantities.

Current Status: The program is operational.

Products to be Issued: The photonuclear data file has been completed up to the end of 1964 and contains about 1500 data sheets. Reprints have been collected for over three-fourths of the original papers. An index to this data has been coded on IBM cards in such a way that computer techniques can be used to produce and maintain a complete cross-referenced bibliography for the data in the compilation. This data index will be published in fiscal year 1966.

Future Plans: The 1965 photonuclear literature will be added to the data file and to the data index. An updated version of the data index will be published toward the end of fiscal year 1966.

The compilation part of the project having been completed, critical evaluation of the data will begin during FY66. This will involve for each nucleus a detailed comparison of all measurements of a given photonuclear reaction. Inverse reaction cross sections will be converted by detailed balance calculations. A close look will be taken at quoted systematic errors and factors influencing their reliability. Relative measurements (e.g., angular distributions) will be normalized with the best available information. It shall be pointed out where apparently equal accuracy data conflict and what new measurements are most needed. The evaluated data will be presented in tabular and graphical form in a manner to facilitate comparison with theoretical calculations. Systematic trends of photonuclear properties as a function of atomic number and mass number will be sought.

IV. ATOMIC and MOLECULAR PROPERTIES

This program area covers a wide variety of specific subjects, all of which are functions primarily of individual atoms or molecules, rather than of some specific state of aggregation. Needs for standard reference data fall generally into two categories -- those concerning basic scientific research or the extension of theoretical understanding, and those concerning technological problems, especially the analysis and identification of materials.

Prior to the activation of the National Standard Reference Data System, there were over a dozen well-recognized, long-term data compilation projects actively working to supply data for one or the other of these needs. The NBS Office of Standard Reference Data has taken over complete or partial support of several of the existing projects, and has initiated another dozen. However, adequate coverage of the whole field is far from reality. Most of the current projects should increase their present budget and staff, and at least another dozen projects should be started as soon as possible to give attention to high-priority topics.

The Atomic and Molecular Advisory Panel, headed by Dr. E. U. Condon of the University of Colorado, had its first meeting in May 1965 at Boulder, Colorado. Membership of the panel is shown in Appendix A.

The Panel listed sixty-three specific groups of properties in the field of atomic and molecular properties (see Appendix B). Twenty-eight of the topics were given high priority, of which, five were judged to be critically and especially urgent.

The OSRD is currently supporting one or more compilation projects in three of these five critical areas; there is at least some compilation effort going on in all five. Of the twenty-eight high priority properties, fifteen are being given some active attention.

The active data compilation projects in the area of Atomic and Molecular Properties are described in more detail below. Projects performed by NBS Technical Divisions are listed first, then NSRDS contract projects, and finally projects supported by other sponsors. In several cases, two or more projects are concerned with the same property or group of properties. With the exception of direct spectral data, there is little or no duplication of coverage. Because of the very widespread use of spectroscopy for analytical and identification purposes, a number of projects have developed over the course of years to supply reference spectra. The Office of Standard Reference Data recognizes a definite (though not complete) responsibility to coordinate such efforts and reduce undesirable overlap.

1. Title of Project: Data on Atomic Energy Levels as derived from Optical Spectra

Principal Investigator: C. M. Sitterley, Atomic Physics Division, NBS

Technical Scope: This activity is concerned with the compilation, critical evaluation, publication and general dissemination of data on the energy levels as derived from optical spectra of atoms and ions; and on the observed transitions giving rise to these levels, term designations, electron configurations, Zeeman effect and general properties of atomic structure.

The data published and otherwise made available to the scientific and technical community constitute some of the most basic constants needed in a variety of fields, such as, plasma physics, astrophysics, atmospheric physics and spectrochemical analysis. Spectroscopic data furnish basic information required to study such problems as stellar evolution, stellar structure, chemical abundances of elements in the universe. Much of the information obtained from rocket and satellite observations is interpreted on the basis of data published by this project; such diverse problems as the diagnostics of rocket exhausts and the analysis of steels depend upon these data.

This project has been given the international responsibility for the compilation, evaluation, publication and general dissemination of data on the energy levels derived from the spectra of atoms and ions and on the observed transitions giving rise to these levels. This responsibility has been delegated by the following organizations:

1) The NAS-NRC Committee on Line Spectra of the Elements
2) The IAU Commission 14: Fundamental Spectroscopic Data
3) The IAU-IUPAC-IUPAP Triple Commission for Spectroscopy
4) The NSRD System

Products Issued: As a long-term compilation project, this activity has published a number of tables, including:

a) NBS Circular 467, Vol. I, II, III, Atomic Energy Levels as derived from the Analyses of Optical Spectra.
b) NBS Circular 488, Sections 1,2,3,4,5, An Ultraviolet Multiplet Table.
c) NBS Technical Note 36, A Multiplet Table of Astrophysical Interest.
d) NSRDS-NBS-3 Section 1, Selected Tables of Atomic Spectra.

Current Status and Future Plans: In addition to maintaining the Reference Data Center for Atomic Spectra, serving a variety of consultative and advisory functions, and following the progress of programs in other laboratories, this project has the following objectives to be realized during Fiscal Year 1966:

1) Compilation and publication of tables on Na I and Mg II and starting work on Ar II, K I and Ca I for Monograph 87, Section 1, Atomic Spectra Selected Tables: Atomic Energy Levels and Multiplet Tables.

2) Complete and publish Monograph 61, the second revision of Rowland's Table of Solar Spectrum Wavelengths. This publication includes some 20,000 lines observed in the solar spectrum between 2935A and 8770A. It is a project promoted by the International Astronomical Union and being carried out in collaboration with M. Minnaert at the Utrecht Observatory in The Netherlands.

2. Title of Project: Critical Tabulations of Atomic Transition Probabilities

Principal Investigator: W. L. Wiese, Atomic Physics Division, NBS

Technical Scope: This activity is concerned with the numerical data for atomic transition probabilities, which determine essentially the intensities of spectral lines. This is the first attempt to undertake a general critical compilation of this material, which is urgently needed by plasma physicists, spectroscopists, and astrophysicists. The specific objective is the critical compilation of atomic transition probabilities from all available literature sources for the lightest ten elements and for selected heavier elements, which

are important for plasma physics, space physics and astrophysics. This project receives all of its financial support from the Department of Defense Advanced Research Projects Agency. Close cooperation is maintained with the NSRDS and with other data projects.

Products Issued or to be Issued: This project has already issued NBS Monograph 50 "Bibliography on Atomic Transition Probabilities"; a compilation of data on the first ten elements has been prepared and is in press.

Current Status: The staff members are now updating the bibliography and are starting a critical compilation of selected heavier elements, to be ready by 1967.

The compilation will be primarily used by physicists, chemists and engineers working in the following fields: (a) Atomic physics and spectroscopy; (b) Plasma physics; (c) Astrophysics; and (d) Space technology.

3. Title of Project: Molecular Ionization Data Compilation

Principal Investigator: H. M. Rosenstock, Physical Chemistry Division, NBS

Technical Scope and Plan of Operation: Accurate information on ionization potentials and general energetics of molecular ionization and decomposition processes is of importance in various areas of science . Existing data compilations are outdated.

Current Status: The present project has accomplished the following tasks:

1. Searched all literature from 1955 to date for relevant information.
2. Devised a standard format for recording the information.
3. Devised an automated scheme for rapid retrieval and printout of any desired information in this field.

Requests for specific information by individuals in government, industrial and academic laboratories are being answered on a same-day basis. Also, a comprehensive body of data on ionization potentials is being made available to J. L. Franklin and F. H. Field, who are planning a critical evaluation of the data.

Future Plans: To maintain the file up-to-date; issue a bibliography and data printout for photoionization; issue annual supplements to the revised critical compilation of Franklin and Field; and establish similar files in ion-molecule reactions, isotopic abundances and atomic reaction kinetics.

4. Title of Project: Atomic Collision Cross Section Data Center

Principal Investigator: Lee J. Kieffer, Laboratory Astrophysics Division, JILA, University of Colorado, Boulder, Colorado

Technical Scope: The Information Center collects published reports which contain low energy atomic data of interest to plasma physicists and astrophysicists. Current and past literature is surveyed in order to obtain a complete bibliography of such data. When it is appropriate, data are compiled and critical reviews are issued.

This Data Center was established with partial support from the Department

of Defense, Advanced Research Projects Agency. ARPA retains a strong interest in the program and in the output of the Center; it still provides support for much of the related experimental program and has supported at least a portion of the program of critical review monographs which are being written by leading atomic physicists on the basis of the compilations prepared by the Data Center.

Current Status: The bibliography of low energy electron collision cross section data is current. A critical review of experimental electron impact ionization cross section data has been completed. A critical review of the data for electron impact excitation of atoms is in progress.

Products Issued or to be Issued: JILA Report No. 4 - A Bibliography of Low Energy Electron Collision Cross Section Data. JILA Report No. 30 - A Compilation of Critically Evaluated Electron Impact Ionization Cross Section Data for Atoms and Diatomic Molecules. JILA Report No. 34 - A Bibliography of Low Energy Electron Cross Section Data, 1964. JILA Report No. 31 - Electron Impact Ionization Cross Section Data for Atoms, Atomic Ions and Diatomic Molecules: I. Experimental Data (to be published in Reviews of Modern Physics, January, 1966). Bibliography of Low Energy Electron Collision Cross Section Data (to be issued as either a JILA Report or NSRDS Report, April, 1966). Compilation of Experimental Electron Collision Cross Section Data (April,1966). Bibliography of Photodetachment, Photo Ionization Cross Section Data, (April or May, 1966).

Future Plans: The immediate future will be taken up with the critical review of the data for electron impact excitation of atoms and the preparation of the above mentioned bibliographies and the compilation of data.

5. Title of Project: Electromagnetic Cross Section Compilation

Principal Investigator: J. H. Hubbell, Radiation Theory Section,
Radiation Physics Division, NBS

Technical Scope and Objectives: To generate and periodically update standard reference tables of photon and related electromagnetic cross sections, over the energy range from about 0.1 keV to beyond 10 GeV for use by scientists and engineers.

To evaluate and incorporate into these tables experimental and theoretical cross section data from the literature and to utilize evaluated data from the NBS Photonuclear Data Center.

To calculate and tabulate, where present accuracy is inadequate, electromagnetic cross sections such as photoelectric absorption, Comptom scattering, pair (and triplet) production and bremsstrahlung, including polarization effects, radiative corrections, and other refinements needed for consistency with measured data.

To serve as information center and coordinator for photon cross section measurement programs at university, government and other laboratories.

Current status: The program is operational.

Products issued or to be Issued: Completion of a program of theoretical calculations related to bremsstrahlung and pair production, resulting in

published results on electron and positron polarization, screening effects in elastic electron scattering, and a review article on electron scattering without atomic or nuclear excitation.

H. Olsen and L. C. Maximon,"Polarized electrons and positrons by tagging technique,"Physical Review Letters 13, 112-114 (1964).

J. W. Motz, H. Olsen, and H. W. Koch,"Electron scattering without atomic or nuclear excitation,"Review Modern Physics 36, 881-928 (1964).

Completion of a numerical evaluation of the combined effects of the radiative correction to Compton scattering and double Compton scattering.

K. J. Mork, "Integrations of the cross section for double Compton scattering and the radiative corrections to Compton scattering," (to be published).

Current knowledge of experimental and theoretical photon cross section data over the energy range 10 keV - 10 GeV was reviewed, and interim tables of these data were compiled for inclusion in the IAEA "Engineering Compendium on Radiation Shielding."

Future Plans: Completion of work on numerical evaluation of triplet cross sections.

Complete the contribution to the "Engineering Compendium on Radiation Shielding."

Continue revision of photon attenuation coefficient tables. Main emphasis will be in the photonuclear region 5-100 MeV utilizing, in addition to the above Compton scattering and triplet results, the pair production calculations now in progress. In addition, revision will be attempted in the region 1-100 keV.

Initiate, where gaps in experimental and theoretical photon cross section data occur, new theoretical calculations.

6. Title of Project: Microwave Spectral Tables

Principal Investigator: Yardley Beers, Radio Standards Physics Division, NBS, Boulder, Colorado
Deputy Investigator: Marian S. Cord, NBS, Boulder, Colorado

Technical Scope and Plan of Operation: The objective of this project is to publish a compilation of the spectral lines of gases lying nominally in the microwave region, which, for the purpose of this project, is interpreted to lie between about 300 mHz to 300,000 mHz. According to the present plan, this compilation will be published in five volumes:

Vol. I Diatomic Molecules
Vol. II Line Strengths of Asymmetric Rotors
Vol. III Spectra of Polyatomic Molecules Capable of Exhibiting Internal Rotation
Vol. IV Spectra of Polyatomic Molecules Not Capable of Exhibiting Internal Rotation
Vol. V Listing of Spectral Lines according to Frequency

Current Status: Volume I was published December 1, 1964, and Volume II was published December 15, 1964. In setting up the remaining three volumes, the procedure involves the heavy use of electronic computers for composition. At the present time, all of the material for Volume III is at hand and ready to be set into type. The computer programming has undergone final debugging. A preliminary computer printout of the spectral lines arranged under the respective molecules has already been accomplished. The introduction has been written and all the possible manual typing has been completed. In Volume IV, the literature has been completely searched and all of the relevant data have been entered onto punched cards, but the punching has not been completely verified. The first draft of the introduction and preface has been completed. Essentially, the same programming will be used for Volume IV as for Volume III, but with minor modifications. Most of the material in Volume V will be taken from some of the same punched cards that were used in Volumes III and IV. However, the spectral lines in Volume I were punched on cards with a different system. New cards, in accordance with the new system, have now been punched. There remains a small amount of programming to sort these cards out in proper order.

Products Issued or to be Issued: The five volumes constitute the complete output of this phase of the Microwave Spectral Data Project. Future activities in this area, including continuing compilation project to maintain an up-to-date collection of values, under the direction of Dr. D. R. Lide of NBS, will be organized with NSRDS support.

7. Title of Project: Atomic and Molecular Processes Information Center

Principal Investigator: C. F. Barnett, Oak Ridge National Laboratory

Technical Scope:

A. Heavy Particle-Heavy Particle Interactions

1. Elastic Scattering Collisions
2. Excitation
3. Dissociation
4. Inelastic Energy Losses
5. Electron Transfer
6. Ionization and Stripping
7. Ion-Ion Recombination
8. Collisional Deexcitation, Broadening and Relaxation
9. Heavy Particle Interchange, Rearrangement and Recombination Reactions
10. Spin Exchange
11. Electron Detachment from Negative Ions
12. Interaction Potentials

B. Interactions with Static or Quasi-Static Electric and Magnetic Fields

1. Excitation
2. Dissociation
3. Ionization
4. Detachment
5. Quenching

C. Particle Penetration in Macroscopic Matter (Ions, Neutrals and Electrons)

1. Energy Losses

2. Energy to Create an Ion Pair
3. Particle Range
4. Multiple Scattering
5. Charge State Populations
6. Excited State Populations

A thorough job in these areas requires awareness of publications in atomic and molecular structure and particle transport in gases.

Plan of Operation: Data are collected and evaluated by competent technical people working in atomic and molecular physics or chemistry. Project personnel are AEC staff scientists who spend 10-50 percent of their time in data analysis and evaluation, and the remainder of their time doing experimental or theoretical work. This effort is augmented by university scientists who are under individual subcontract with the Information Center. Because the work is so closely related to the continuing AEC programs for experimental and theoretical work, the project is jointly supported by AEC and NBS. The output is especially useful to AEC staff scientists and contractors.

A fully automatic machine storage system has been inaugurated to replace earlier hand operations. The literature is searched by the technical staff and the pertinent references are key punched directly onto computer cards. The cards are processed to serve as a working bibliography. This printout is then assigned to specialists who read the papers, make preliminary evaluations, index and classify each paper and note information such as reactants, particle energy regions, etc. This information is then punched onto the original reference card, which is then printed out by categories and in a form suitable for reproduction. Also, the information contained on the cards is transferred to magnetic tape for retrieval by title words, categories, reactants, authors, or any combination of these.

At periodic intervals, the papers will be reassessed or reevaluated. Useful data will be extracted from graphs by automatic analog to digital conversions and then to magnetic tape. Attempts are being made to enlist the author's aid in supplying tabulations of the original data. The tabulations, both from authors and machine extracts, will be published along with critical comment from the reviewer.

Current Status: Preliminary scanning and evaluation has been completed of the literature since 1963. Some of the major contributing journals, such as Physical Review, Journal of Chemical Physics, etc., have been searched back to 1950. The initial phases of our machine information storage phase have been tested and have proven to be adequate. At present, 2,000 references are being placed into 7090 computer to serve as a base for testing the accuracy and completeness of machine retrieval. The retrieval program is being written in a universal language so that the input can readily be changed from one computer to another.

Products Issued or to be Issued: In August, 1965 the first bibliography (1963) for the Information Center was issued as AMPIC-1. An international directory (AMPIC-2) has been distributed to the technical community. The second bibliography, issued as AMPIC-3, covers literature for the year 1964.

Future Plans: Development of machine techniques to handle data. The entire manual system is at present being converted to computer operation. Experiments will be continued to study the efficiency and feasibility of mass storage and retrieval, especially for tabular and graphical data.

Reviews and tabulations were started early in 1966. Three topics were chosen for the first reviews: (1) Ion and atom interchange reactions; (2) Ionization by heavy particles; and (3) Particle interactions with electric and magnetic fields. The manuscript of the first review is about 40 percent complete. A proposal for the second has been received.

Present plans are to include particle interactions with surfaces beginning early in the 1967 fiscal year.

8. Title of Project: Tables of Critically Evaluated Gas Dipole Moment Data

Principal Investigator: Ralph D. Nelson, Jr., Middlebury College, Middlebury, Vermont
David R. Lide, Jr., NBS, Washington, D.C.
Arthur A. Maryott, NBS, Washington, D.C.

Technical Scope: The study consists of the evaluation of all reported measurements of electric dipole moments for molecules in the gas phase. Measurements involving the liquid or solid phases will not be considered because they involve assumptions and interactions of poorly defined magnitude. The project is a revision of NBS Circular 537, by A. A. Maryott and F. Buckley, published in 1953, which is both out of print and out of date. The original literature reports are being obtained for all measurements and will be evaluated by competent workers in the field (the investigators).

Stage I is the compilation of a bibliography listing all reported measurements. Rather than making a costly page by page search through Chemical Abstracts, the results of previous compilers in various areas have been combined. This affords a roughly threefold search through Chemical Abstracts by independent groups of dipole moment data compilers.

Stage II is the evaluation of the original reports and the assignment of a best value to each compound. An estimate of the reliability of the value will be included. Additional information, such as direction of the dipole moment and the dipole moment in excited vibrational states will be included where appropriate.

Stage III is the preparation of tables, introductory material, and descriptions of precision calibrations for experimental appartus. Publication follows.

Current Status: The first stage is complete. Two copies of the bibliography cards have been made, to avoid loss in handling. Spot checks of Chemical Abstracts have proven that the compilations used were thorough and complete. It is estimated that Stage II will be completed by next May or June, and Stage III by September 1966.

Products to be Issued: A monograph similar to Circular 537 will be prepared. In addition, a set of punched cards containing the bibliography and the finally selected best values will be prepared to facilitate future revisions and to allow for computer handling of the material.

Future Plans: The bibliography will be retained in card form for easy up-dating under later phases of this project. A revision of the tables will be considered when the mass of new material justifies such work.

Need for the Results: The experimental values of electric dipole moment are used by theoreticians to confirm their predicted electron density calculations and to predict intermolecular dipole interactions. Their work will be more effective if a best value, chosen by competent scientists familiar with all the various experimental methods, is available.

9. Title of Project: Bibliography on Flame Spectroscopy

Principal Investigator: Radu Mavrodineanu, Phillips Laboratories, Briarcliff Manor, New York

Technical Scope: To assemble references of published works in the field of flame spectroscopy with special emphasis on the analytical aspect, and present the information in the form of a collection following the plan summarized below.

Flame Emission

1. Review of sources of material
2. Fundamental works -
   Flame analytical, flame geometry and composition, flame temperature, flame reactions, molecular species.
3. Instrumentation
4. Analytical Procedures
5. Less familiar combustion flames
6. Electrical discharges having the appearance of combustion flames - RF - discharges, blown arcs, arc and spark-in-flame

Flame Absorption

1. Fundamental works and reviews
2. Hollow cathodes

Current Status: About 500 references have been collated, typed on punched cards, indexed and organized according to the foregoing plan.

Products issued or to be issued: A typed manuscript has been submitted for publication by the National Bureau of Standards.

Future Plans: It is the intention of the investigator to keep the assembly of references work on flame spectroscopy up-to-date.

10. Title of Project: Atomic Cross Section Data Review Program

Coordinator and Editor: E. U. Condon, University of Colorado

Technical Scope: A series of review articles and monographs has been scheduled, based on the data compiled on particle cross sections for collisions with electrons. The compilation is done by the Atomic Cross Section Data Center at the Joint Institute for Laboratory Astrophysics. Authors of individual review articles are selected for their scientific competence in the specific field to be covered. At least one of the data compilers at the Data Center works as a co-author. Dr. E. U. Condon serves as editor of the series and provides general scientific coordination and assistance. Some of the titles in this series will be supported by the Advanced Research Projects Agency of the Department of Defense under a contract with NBS. ARPA also provides support for related measurement programs which furnish some of the data input to the Atomic Cross Section Data Center. The review articles provide for discussion of related theories, interpretation of data, and general analysis of the state of quantitative knowledge in this area.

Products Issued or to be Issued: The first review, "Electron Impact Ionization Data for Atoms, Atomic Ions and Diatomic Molecules," is now available as JILA Report No. 51, and will appear in the January 1966 issue of Review of Modern Physics.

Current Status: A contract has been written to provide the services of B. L. Moiseiwitch of Queen's University of Belfast, as principal author. The topic will be Electron Inelastic Scattering Cross Section Data for Atoms.

Future Plans: Additional reviews will be prepared based on data compilations issued by the Atomic Cross Section Data Center. A schedule of one review per year is planned.

Customers: Astrophysicists, physicists, astronomers and other scientists active in space and defense programs will use these reviews.

11. Title of Project: Compilation of Standard X-ray Wavelengths

Principal Investigator: J. A. Bearden, Department of Physics,
Johns Hopkins University

Technical Scope: Under related experimental programs, J. A. Bearden has succeeded in improving the accuracy and precision of techniques for measuring and recording X-ray intensities and angular distributions. Using such high-accuracy data, he will recalculate and redefine an absolute scale of X-ray wavelengths, and prepare an improved compilation of wavelength data. He will also be able to calculate improved values for the h/e ratio, and thus make better determination of several fundamental constants.

Products to be issued: A compilation of X-ray wavelengths will be published as a revision of AEC Report NYO 10586, "X-ray Wavelengths," by J. A. Bearden.

Current Status: Sources of error and inconsistency in earlier compilations have been defined, and the major effort is being directed to recomputation of numerical values based on existing measurements. At the same time, the parallel

experimental program is being developed (under other sponsorship) to provide new data.

Future Plans: In addition to the compilation of a standard scale of X-ray wavelengths, the investigator will establish better criteria for defining wavelengths. Future compilations will be easier to prepare and will be more reliable.

12. Title of Project: Molecular Fundamental Vibration Frequencies

Principal Investigator: T. Shimanouchi, Department of Chemistry, University of Tokyo

Technical Scope: Using high resolution spectroscopy, far infrared spectroscopy and normal coordinate analysis, Dr. Shimanouchi is computing fundamental vibration frequencies of a series of classes of chemical compounds--especially organic compounds with selected deuterium substitution. The resulting values are tabulated with assignments to modes of vibration, accompanied by indication of reliability and probable error.

Products Issued or to be Issued: Tables presenting results for fifty-nine selected molecules have been prepared and will be published as a Monograph in the NSRDS-NBS series. A second group of tables is now being prepared.

Current Status: The text of the first monograph is in press. Computation and compilation of values for the second series of compounds is approximately fifty percent complete.

Future Plans: The first monograph will appear by about July 1966. Tables on the second series of compounds will be completed by September 1966, and should be published by early 1967. A continuing project is deemed desirable, since data of this type are needed for a substantial number (several hundred) key molecules; uniformity of treatment is very important.

Customers: Tabulations of fundamental vibration frequencies provide better understanding of thermodynamic properties, calculation of molecular energy levels, and accurate knowledge of molecular form fields, chemical bond strengths molecular structure. Scientists working in all these fields will use the tables.

13. Title of Project: Study of Needs and Quality Standards for Infrared Spectral Compilations

Principal Investigator: Nelson Fuson (President of The Coblentz Society, Inc.) Fisk University, Nashville, Tennessee

Technical Scope: Several sources of Infrared Spectral Data for reference purposes already exist. Under other projects, the NSRDS has developed plans to compile and publish additional reference spectra. It was recognized, therefore, that activities in this area must take account of the needs for reference spectra and adhere to adequate quality standards for the process of selection and evaluation of spectra, to the end that NSRDS products are useful, scientifically accurate, and not a duplication of existing collections. The Board of Management of the Coblentz Society was asked under the terms of this project, to

study needs for Infrared Spectral Data, to define quality standards for compilations of spectral data, and to provide a professional basis for compilation plans in several categories of user requirements.

Products Issued or to be Issued: The recommendations of the Coblentz Society Board of Management have been summarized in a report which has been submitted to an appropriate technical journal for publication. Reprints of the report will be obtained by OSRD for further distribution.

Current Status: The summary report defines three categories of IR spectra and sets forth criteria for all three categories. This report completes the first phase of the cooperative effort of The Coblentz Society Board of Management with the OSRD.

Future Plans: The Coblentz Society Board of Management will meet two or three more times in the next year, and will follow-up on the application of their recommendations to the OSRD. The OSRD has already made plans to incorporate the results of this study into other compilation projects concerned with infrared reference spectra. Responsibility for compilation activities in the three separate categories of spectra which the Coblentz Society has recognized will be assigned to bodies which are appropriately concerned with such information.

Customers: The summary report will be used directly by the OSRD staff and by those spectroscopists associated with it who are collecting, evaluating and planning to distribute Infrared Spectral Data under other NSRDS projects. Indirectly, all those who use Infrared Spectroscopy for analytical, identification or structural analysis purposes will gain, because these projects will be more closely keyed to their needs.

14. Title of Project: Infrared Spectral Data for Reference Purposes

Principal Investigator: L. E. Kuentzel, Wyandotte Chemical Company, Wyandotte, Michigan
S. Etris, ASTM, Philadelphia, Pennsylvania

Technical Scope: Infrared Spectroscopy is widely used for analytical and identification purposes in industrial, academic and government laboratories. Effective use of Infrared Spectroscopy in this way requires standard reference spectra of reliable quality. There are already several sources of reference spectra available on a commercial, semi-commercial or non-profit basis. However, there is a growing need for new reference spectra covering additional classes of compounds, as well as a need for reference spectra of higher quality to take full advantage of improved instrumentation in this field. This project has the mission of collecting, evaluating and distributing Infrared Spectral Data of good quality adequate for identification and analysis purposes. In particular, attention is being given to collection of Infrared Spectra from a number of government agency laboratories and private industrial laboratories which could

be made available to the public if a suitable distribution means were provided.

Products Issued or to be Issued: Infrared Spectral Data sheets will be issued, probably through the offices of the ASTM, in the form of loose-leaf sheets, one spectral data curve to a page. Present plans are that these loose-leaf data sheets will be distributed in groups of similar or related chemical compounds. Indexes to these compilations and unit collections will be provided by the ASTM as part of their own program for indexing spectral data.

Current Status: More than a thousand spectral curves have been collected from a number of laboratories. The cooperation of a substantial number of other laboratories has been solicited and promised. In order that the evaluation procedure can be performed efficiently, it is necessary that several reference spectra on the same substance be collected and available at a single time. To achieve this purpose, the current emphasis in the program is on the collection of additional spectra to be put through the evaluation procedure.

Future Plans: Collection of Infrared Spectral Data from appropriate laboratories will continue. Evaluation of these spectra will be performed as adequate collections become available, and the procedures developed by the Coblentz Society Board of Directors under a separate project already described will be applied. Publication of these spectra will be effected as appropriate blocks of spectra on related chemical compounds become available.

Customers: Infrared Spectroscopy is at present the most widely used single instrumental analytical technique in the United States chemical industry. Reference spectra are needed by all people who use Infrared Spectroscopy as an identification and analytical method.

15. Title of Project: Compilation of Atomic and Molecular Gas Laser Transitions

Principal Investigator: W. R. Bennett, Department of Physics, Yale Univ.

Technical Scope: Certain data on gaseous atoms and molecules, notably energy levels and transition wavelengths, together with associated ambient conditions, are highly useful in the design and interpretation of gas laser experiments. This project is intended to provide uniform tabulations of such data on a continuing basis. The data will include numerical indications of the transitions which can be stimulated, the wavelength of the resultant light, the appropriate pressure for efficient operations, plus gain, power, etc., of the systems.

Support for this project is provided by the Department of Defense Advanced Research Projects Agency through a contract with NBS. ARPA maintains a strong interest in compilations of data related to atomic and molecular energetic processes.

Products Issued or to be Issued: Tabulations containing the results of this work will be published and distributed by the principal investigator at three to six month intervals as the data accumulate. Distribution will be made informally to those workers who are known to be active in the field. At appropriate intervals, probably annually, the NSRDS may issue a monograph containing those data sheets prepared up to that time.

Current Status: A first distribution, containing a summary of transitions on which optical oscillation has been obtained, is being prepared for distribution by Dr. Bennett.

Future Plans: Data sheets will be distributed periodically. It is anticipated that this project will be a continuing one, so that the developing technology in this field can be kept up-to-date and users of the data may have a source of reliable tabulations.

Customers: Physicists, astro-physicists and electronic scientists and engineers active in research and development on laser systems will use such data to provide more efficient, economical and reliable planning and interpretation of their work.

16. Title of Project: Tables of Ionization and Appearance Potentials

Principal Investigator: J. L. Franklin, Department of Chemistry, William Marsh Rice University

Technical Scope: A compilation is being prepared of critically evaluated ionization and appearance potentials and related thermodynamic values. In one sense, this project is an up-dating and continuation of the tabular material in the well-known text "Electron Impact Phenomena" by Franklin and Field, published by Academic Press in 1957.

The authors are using the bibliographic material collected in the NBS Mass Spectrometric Data Center (project #3 above).

Products to be Issued: The tables will be published through NBS and GPO channels.

Current Status: About one quarter of the available references have been surveyed, and several tables have been drafted.

Future Plans: Analysis of the references and preparation of the tables will continue. The manuscript should be completed toward the end of 1966.

Customers: The tables will be widely used by mass spectrometrists and by many scientists in other fields, including atomic and molecular collision physicists, thermodynamicists, kineticists and analytical chemists.

SUPPLEMENT TO ATOMIC AND MOLECULAR PROPERTIES

The data compilation projects listed above are all operating with the direct cognizance of the National Standard Reference Data System. In every case, except one, they derive all or a fraction of their financial support from the NSRDS. In addition, there are several data compilation projects concerned with atomic and/or molecular data under other sponsorship, which have only informal association with the National Standard Reference Data System. In some cases the structure and mission of these projects makes their continued independent operation desirable; in other cases it will probably be appropriate for the Office of Standard Reference Data to develop a closer association between the individual projects and the System.

Independent data compilation activities are of particular interest in the following areas:

1. The National Academy of Science-National Research Council Committee on Fundamental Constants serves as the United States expression of national interest on the definition of the values of fundamental constants and as the affiliated organization for international consideration on this subject. A report of the NAS-NRC Committee on Fundamental Constants was published as an NBS Technical News Bulletin in October 1963. It contained a tabulation of the recently accepted international values for the Fundamental Constants.

2. Molecular spectra widely used throughout industry and academic research, derive much of their usefulness from collections of reference spectra used for comparison. A number of organizations currently publish reference spectra in one or more specific fields. Some are commercial enterprises, others are essentially non-profit or cooperative in nature. These sources of reference data serve a valuable purpose and the plans of the Office of Standard Reference Data take account of their continued operation. These sources provide data in infrared and raman spectra, visible and ultraviolet absorption spectra, nuclear magnetic resonance spectra, and mass spectra.

3. Several excellent text and reference books are available dealing with molecular energy levels derived from spectral data. In many cases, these text books are written by outstanding scientists and contain some tables of reference data of high quality.

4. There are also text books which provide tables of data pertaining to individual or bulk properties of atoms, molecules and ions. Subjects covered by these texts include interatomic distances and configurations, dipole moments, dielectric constants, refractive indices and atomic and molecular polarizabilities.

5. There are numerous reference and text books dealing with semi-quantitative data such as gas chromatographic values, differential thermal analysis and similar topics.

6. There are several comprehensive data compilation and publication programs which provide important parts of present reference data libraries. These include the volumes of Landolt-BornsteinTabellen, the Tables de Constantes et Données Numerique distributed by Pergamon Press, the Smithsonian Physical Tables and the Handbook of Chemistry and Physics.

V. SOLID STATE

The first solid state panel meeting was February 8-9, 1965. The panel consisted of twelve members, divided evenly between government, university, and industry. Panel members are listed in the Appendix.

The panel identified those properties which were considered to be in the domain of solid state. It prepared a list of those properties which were amenable to compilation and for which sufficient meaningful data were available to warrant compilation. Some 28 properties (subjects) were so identified. As a result of this panel meeting several people were contacted for their interest to initiate compilation of data in the area of their scientific domain and several programs were initiated.

In addition, the panel was advised of those compilation activities which were known to be in operation. Tentative identification of possible activities qualifying for the NSRDS were made.

A. Activities supported by OSRD

1. Diffusion in metals and alloys. This is a project that will provide meaningful data on diffusion in metals and alloys, as a part of a larger program on diffusion in solids.

Principal Investigator: J. Manning, National Bureau of Standards

Properties Covered: Diffusion coefficient, activation energy

Product: No product issued to date; however, a bibliography will soon be available. Future products will be tables of data of diffusion coefficient and activation in energies.

Status: Literature search is just about completed and critical evaluation of extracted data will begin this fiscal year.

Future Plans: This is a continuing project and the data will be maintained on a current basis.

2. Alloy Data: This modest program was initiated to determine the availability of any existing sources of compilations of metals and alloy data. These sources include handbooks, bibliographies, conference proceedings, and text books containing extensive compilations of alloy data. The range of information sought is: (a) equilibrium phase diagrams as a function of composition, temperature, and pressure, (b) crystallographic data and X-ray lattice parameters, (c) thermodynamic data, (d) selected kinetic data, including diffusion constants, (e) important physical properties such as thermal conductivity, specific heat, magnetic resonance data, and other such data. A compilation of these compilations is being prepared together with brief annotations on each entry.

Principal Investigator: L. H. Bennett, National Bureau of Standards

Status: Literature survey is essentially complete and annotations are

being prepared and a draft being prepared.

Product: An annotated bibliography of alloy data compilations will be published as part of the NBS National Standard Reference Data series.

Future Plans: If funds are available, the effort will be directed to produce an encyclopedia of alloy data. This encyclopedia would summarize data in the areas listed above. It would provide complete data when they are not available in critically evaluated form elsewhere; the encyclopedia would refer the reader to other reviews or compilations for the complete data when such existing compilations are acceptable as critically evaluated and when they are readily available. Effort would be limited to binary and selected ternary alloys, omitting mechanical properties and engineering data.

3. Publication of "Crystal Data": The function of this project is to revise and bring up-to-date, the volume, Crystal Data. This book contains crystallographic data on all solids on which, at least, unit cell dimensions have been measured. The information is used in identifying crystal phases, and as an index to physical properties and structure.

In this revision for the 3rd Edition, the data are to be put on linofilm tapes and magnetic tapes so that future revisions, additions, and corrections may be made quickly, thus promoting currency. A computer program is being written which will allow ready insertion of new data, re-indexing, etc. In a sense, this project is an experiment to determine the feasibility of using a computer program for the rapid revision of a compilation.

Principal Investigators and Location:

1) Chief Editor - Dr. J. Donnay, Johns Hopkins University, Baltimore, Md.

2) Washington Editor - Dr. Helen M. Ondik, Section 313.06, INR, NBS

3) Organic Editor - Dr. O. Kennard, Cambridge University, Cambridge, England

4) H. F. McMurdie, Chief of Section 313.06, NBS, is in general charge of arrangements.

Properties Covered: Unit cell dimension, density, ratios of crystallographic axes, bibliography.

Product: The 3rd Edition of Crystal Data will be published in 1966.

Status: The work is in process. Most of the new material to be added has been identified and edited. The process of putting material on tapes and correcting them is about 1/3 done. Codes are being produced by an outside contractor for processing the magnetic tapes.

Future Plans: It is planned to continue Crystal Data into future editions and possibly to extend its coverage.

4. Standard X-ray Powder Patterns: This is the ASTM program for the Joint Committee on Chemical Analysis by Powder Diffraction Methods. The Committee is composed of members from the ASTM, ACA, and British Institute of Physics. The project is a compilation of diffraction patterns from many sources. This is a part of a new series of NBS Publication, Monograph 25. The financial support

for this project is by the National Bureau of Standards.

Principal Investigator: (For Monograph 25) H. E. Swanson

Properties Covered: Principal lines and intensities

Product: Monograph Series No. 25

Status: Continuing project. When sufficient data have been obtained a new section of the monograph is published.

5. High Pressure Data: This project is concerned with the collection and critical evaluation of all high pressure data (of solids).

Principal Investigator: H. Tracy Hall, Brigham Young University

Properties Covered: High pressure, fixed points, M. P., phase transitions, magnetic electrical and optical properties, thermodynamic data.

Product: No product issued to date. Contract initiated September 1965. Future product will be compilation of high pressure data plus bibliography.

Status: Literature search to obtain a complete bibliography on high pressure data. This will include copies of original articles plus translations when needed.

Future Plans: Continuing project, data file and bibliography will be maintained current.

6. Superconductive Materials: The Standard Reference Data Center on Superconductive Materials will collect and collate all known data on superconductive materials within the capabilities of the present effort. Sources of data will include the published literature as well as unpublished contributions from established research workers in the field. The most probable values of the superconductive constants will be chosen for an ideal material when sufficient data have been published. However, all the data contributions will be referenced, except in a few isolated instances, so that subsequent re-evaluation may be made by the research worker utilizing the data on a specific material. Divergent values of equal weight will both be listed and referenced.

The basic data will be maintained in readily accessible hand written form on standard machine cards. The filing will normally be alphabetical by the elements.

Basic data punched on the cards are: (a) the elements present; (b) the critical temperature; (c) the critical field; (d) a literature reference; (e) the lowest temperature to which a nonsuperconductive material has been tested; and (f) the Strukturbericht code for the crystal structure.

All of the above are also hand written on the cards as well as (a) complete crystal structure data where available; (b) the composition of the alloy, compound or mixture; (c) available thermodynamic data (electronic specific heat

and Debye theta); (d) data on high field (or Type II) superconductors and (e) additional comments where pertinent.

Computer programs have been written to introduce the punched data on the cards onto tape for fast sorting and collation. Printout may be by alphabetical element sequence, by critical temperature value, by critical field value and by specific element -- i.e., all materials containing tin.

Principal Investigator: B. W. Roberts, General Electric Company, Schenectady, N.Y.

Properties Covered: Critical temperature, critical field, temperature range, crystal structure, composition, thermodynamic data.

Product: A compilation has been issued, "Superconductive Materials and their Properties," published in "Progress in Cryogenics." An addendum to this publication will be issued in May 1966.

Status: The main file has been updated and the crystal structure code added. The literature has and is being systematically searched. New data are being extracted, recorded and matching cards punched.

Future Plans: Literature will continue to be searched and a new addendum to the above article issued until such time when the accumulation of data warrants the publication of a monograph.

B. Projects supported by Other Agencies

1. Diffusion in Gases, Liquids and Solids: This is a comprehensive program funded entirely by NASA that essentially rounds out a complete compilation program in diffusion. The other parts of the diffusion program are, metals (NBS), semiconductors (IBM), oxides, carbides, nitrides (LRL), the latter two compilations are discussed below.

This project consists of four separate compilations:

Diffusion in turbulent systems: (Dr. J. M. Marchello)

Data on the transport of chemical species, heat, and momentum in turbulent flow fields is being compiled and evaluated. Both confined and free flow fields are being surveyed. Some of the types of transport in confined flow are: heat, mass and momentum transport in conduits; porous media, and boundary layers. Free or unconfined flow includes: jets and streams issuing into large bodies; meteorological, and oceanographic flows.

Only systems for which the molecular transport coefficients are well established are being considered. Excluded from the survey are: non-Newtonion fluids; systems at extremely high or low temperature; magnethohydrodynamic systems; and, very low pressure gases. The major emphasis at present is on subsonic turbulent flow of gases and liquids. Some information is becoming available on turbulences in supersonic flow of gases. As more information becomes available supersonic flow fields will be given increased consideration.

The plan of operation will follow a three step sequence: (1) define the quantities to be measured and the interrelationship between the basic statistical

turbulent properties and the turbulent transport coefficients; (2) survey the literature in each of the areas to determine what information and data are available; (3) critically evaluate data and present it in convenient form for use by workers in the field.

Diffusion in Gases: (E. A. Mason)

Collection and critical evaluation of all the measurements of gaseous diffusion coefficients at all available temperatures in the low-pressure (ideal gas) region. The major emphasis is on binary mixtures; extension to multicomponent diffusion is fairly simple because it is primarily characterized by the binary coefficients of all the pairs in the mixture.

The initial restriction to ideal gases is made because an accurate kinetic theory is available for this region. This theory makes possible an extensive correlation with other mixture properties, in particular the viscosity, the thermal conductivity, and the thermal diffusion factor. The second phase of the project will be to collect such related data and carry out a correlation. The third phase will be to use the kinetic theory to obtain information on the forces between pairs of unlike molecules from the experimental data, insofar as this is practicable.

Diffusion in Liquids: (R. B. Beckman)

Both aqueous and non-aqueous solvent systems with ionizing and non-ionizing solutes are included in the compilation and evaluation program. Excluded initially from this compilation and evaluation survey are those systems in which the solvent or the solute represents a heterogeneous chemical species that can not be readily characterized on the basis of pure component properties -- i.e., a liquid tar or broad spectrum liquid petroleum of generally variable composition and/or properties would not be included, but a binary, ternary or multicomponent mixture (either solvent or solute) of pure components with a definable composition is to be included. Essentially this restriction implies that those systems of well definable composition and bounding conditions for the evaluation of the liquid phase transport properties are of primary interest.

Diffusion in Inorganic Crystals: (H. Schamp)

Compilation will be limited to diffusion in well defined inorganic crystals.

Principal Investigators: J. M. Marchello, H. Schamp, E. A. Mason, R. Beckman, University of Maryland, College Park, Md.

Properties covered: Diffusion coefficient, activation energy, viscosities, mobilities.

Product: No product issued to date. Contract initiated July, 1965. Future product will be tables of data with appropriate bibliography.

Future Plans: This is a continuing project supported by NASA and it is expected to slowly evolve as a major data center in this area.

2. Diffusion in Semiconductors: This project was initiated by the principal investigator's personal interest and was intended originally to be a review article. After discussion with OSRD it was decided that the project would continue

to function as a data center maintaining a current data file. This project is supported entirely by IBM.

Principal Investigator: R. F. Peart, International Business Machine Co.

Properties covered: Diffusion coefficient, activation energies, densities on semi-conductor materials.

Product: None issued to date.

Status: Data is being extracted from the literature and a bibliography will be available next year. It is expected that a monograph containing the evaluated data and discussion will be available within 12 to 18 months.

Future Plans: Indefinite

3. Diffusion in Oxides, Carbide and Nitrides: This is a program initiated in the Inorganic Materials Division of LRL at Livermore and is supported entirely by AEC.

Principal Investigator: R. H. Condit

Properties covered: Diffusion coefficients, activation energies, densities

Product: No product issued to data

Status: Literature is now being collected. Data evaluation will begin sometime in FY 1967.

Future Plans: Uncertain.

VI. THERMODYNAMICS

The Office of Standard Reference Data (OSRD) in developing its program in thermodynamics has relied very heavily on advisory panels, ad hoc panels, consultants, and Bureau personnel. Two conferences under the auspices of the National Academy of Sciences have been held, one in May 1964 and the other in April 1965, both organized by the Office of Critical Tables of the NAS-NRC. These conferences were for the purpose of providing guidance as to the needs of the scientific and technical community for compilations of thermodynamic data and to suggest a priority list of projects. The recommendations resulting from these conferences were carefully screened in light of available funds and personnel and, where possible, action was taken to institute compilation programs.

The Office of Standard Reference Data has made a detailed survey of known data compilation centers funded by other government agencies, as well as those by NBS. In addition to compilation centers, OSRD has attempted to compile a comprehensive list of individuals who are engaged in compilation activities. Most of these compilers are engaged in preparing texts or review articles and they represent a large source of prospective compilation centers.

The OSRD has now identified sufficient groups, some active and others in the category referred to above, which could provide 80-90% coverage of the technical scope in the area of thermodynamics. By this it is meant that 80-90% of data needs for the scientific and technical community could be met by existing groups plus other individuals or groups who have been identified and who have expressed a willingness to engage in compilation activities. To accomplish this coverage would require a considerable expansion in level of effort of many of the existing groups. Such a comprehensive program can be put into effect in an orderly manner as funds become available. An instructive example providing some idea of the unevaluated data accumulating each year may be found in the IUPAC bulletin for thermodynamics and thermochemistry. In the 1962 issue this Bulletin listed 499 references; in 1963, 1282; in 1964, 1819; and in 1965, 2167. In each case the Bulletin gives the literature for the previous year, i.e., the 1965 issue lists the literature for 1964. Only a certain fraction of this literature appears in compilations; the remainder is dispersed throughout the world literature.

Additional activities which are needed to give adequate property coverage for data needs in thermodynamics are:

1. P-V-T relations and all derived data in single and multicomponent systems, including homogeneous and heterogeneous systems (vapor-liquid, solid-vapor).

2. Dissociation constants of acids and bases, and stability constants of complex ions.

3. Half-wave potentials.

4. Solubilities of all substances in aqueous and non-aqueous media (except metals) and all derived data.

5. Bond dissociation energies.

6. Thermodynamic functions as a function of temperatures for all organic substances.

In the following pages are listed those major compilation centers which are now active and whose products contribute significantly to the total data compilation resources of the American technical community. The operations of all these groups involve some degree of critical evaluation. Judgment on whether the designation "Standard Reference Data" should be applied to the products must await the development of an agreed-upon procedure for making such a decision.

INORGANIC COMPOUNDS

Current activities in the U. S. on the compilation of thermodynamic properties of inorganic compounds cover the scope of desired properties reasonably satisfactorily. However, the total level of effort is not adequate and it is estimated that only about one quarter of the published data is evaluated and compiled, thus producing an enormous backlog.

Cooperation among existing compilers is good and consideration is being given to the mechanics of sharing the task of literature searching in this area. A possible mechanism is to confine the task to one laboratory with the other laboratories having remote access to the collected information (bibliography, original documents, tables, etc.). This approach is probably feasible for this area, although it may not be for others.

A. Compilation Centers Supported Entirely by NBS-OSRD

1. Selected Values of Thermodynamic Properties of Inorganic Substances, Revision of NBS Circular 500, Series I. This project, in the past, has been supported largely by the AEC and, indeed, this agency will have covered the major cost of the revision. The project is now entirely supported by NBS-OSRD.

Principal Investigators: D. Wagman and W. Evans, V. B. Parker, I. Halow, S. Bailey, and R. H. Schumm, National Bureau of Standards.

Properties Covered: Standard Gibbs Energy, Heats of formation, Entropy, Heat capacities, Enthalpy at absolute zero, and Thermal Functions.

Product: Tables of selected values of the properties of standard states of the elements and their compounds.

Status: The first portion of revised tables of heats and free energies of formation at 298.15°K, for the first twenty-three elements in the standard order of arrangement, have recently appeared as NBS Technical Note 270-1.

Future Plans: Tables for the next nine elements are completed and typed. These will be submitted for publication as TN 270-2. Additional tables will be assembled and published in the Technical Note Series, as prepared. It is hoped that this revision (of Tables of Series I of C-55) can be completed by next summer. The revision of tables on the heats of phase transitions (Series II Tables) and preparation of the text material relative to the data on Series I are next on the schedule.

Comments: At present the technical staff doing critical analysis of the data consists of six technically trained people. An additional four people are engaged in abstracting current literature, maintaining microfilm reference files, etc. An annual Substance-Property Index to the published literature in chemical thermodynamics is prepared for publication in the Bulletin of Thermodynamics and Thermochemistry, sponsored by the IUPAC.

2. Selected Values of Thermodynamic Properties of Inorganic Substances, Revision of Circular 500, Series II, compilation by same group described in Item 1.

Properties: Heats of transition of all substances (organic and inorganic).

Status: Data are being collected. Critical evaluation and publication depend upon the recruitment of staff and the availability of funds.

3. Thermodynamic Properties of Elements and Compounds, Phase Relations, and other data of general usefulness for correlating physical properties. This program is carried on by L. Brewer of the University of California at Berkeley, and represents a wide range of interests. Most of the compilations are published in the open literature. Project is funded by AEC.

Principal Investigator: L. Brewer, University of California at Berkeley.

Properties Covered: Thermodynamic, spectroscopic, crystallographic.

Product and Status:

a. Thermodynamic Properties of the Elements: The compilation of enthalpies of sublimation and free energy functions of the elements has been a continuing activity since 1944. The first compilations were issued as Manhattan District Project Reports and revised in 1948 for publication in the

National Nuclear Energy Series, Vol.19B. The compilations were brought up to date in 1955 and again in 1958 and were issued as UCRL reports which were not published elsewhere as they are incorporated into JANAF Tables. Data are now reported in R. R. Hultgren's Thermodynamics of Metals and Alloys.

b. Thermodynamic Properties of the Halides: Manhattan District Project Reports were revised and published in the National Nuclear Energy Series, Vol. 19B and have recently been brought up to date in two Chemical Review papers dealing with monohalides and dihalides. No new compilations are in progress that deal with halides alone.

c. Thermodynamic Properties of the Oxides: Manhattan District Project Reports were revised and published in a 1953 Chemical Review paper. The dioxides were brought up to date in a Chemical Review paper in 1961 and the monooxides have been brought up to date in a paper that should be published in Chemical Review in 1966.

d. Thermodynamic Properties of the Actinides: Papers covering the compounds of U, Np, and Pu were published in National Nuclear Energy Series Vol. 14B and in Vol. 1 of Chemistry of Uranium. No compilations are underway at the moment.

e. Thermodynamics of Refractory Compounds: A review was published in National Nuclear Energy Series Vol. 19B and supplemented with additional compilations, particularly for borides and silicides, in Journal of Electrochemical Society 1955 and 1956 and in UCRL-2888. An additional compilation is in progress for refractory intermetallic compounds.

f. Spectroscopic Data: A compilation of excited electronic levels of diatomic molecules was completed in 1962 and published in 1965. Additional compilation along these lines is in progress.

g. Crystal Structure Data: A compilation of structures and composition ranges of the phases of the multicomponent transition metal phase diagrams was published in 1965. Additional compilations for other systems are on hand. No plans as yet for publication.

h. Thermodynamics of Mo Compounds: A compilation on Mo compounds has just started, but will probably take more than a year to complete.

i. Thermodynamics of Aqueous Salt Solutions: Data have been collected for over 25 years. Tables published in 2nd Ed. of Lewis and Randall and will be revised and up-dated.

j. General Thermodynamic Compilations: Compilations in 2nd Ed. of Lewis and Randall will be brought up to date.

4. Low Temperature Heat Capacity. This is a compilation and critical evaluation of all low temperatures (0 - 400°K) heat capacities. It is intended to cover all pure substances (inorganic and organic). This is a low-level effort and progress will be slow unless the activity is increased.

Principal Investigator: G. Furukawa, National Bureau of Standards.

Properties Covered: Heat capacity constant pressure (0 - 400°K).

Product: No product has been issued to date. It is anticipated that the first product will be issued some time during FY66. This will be the heat capacity of alkali metals. In addition, a general bibliography will be made available to interested parties. This work is coordinated with the Thermophysical Properties Research Center at Purdue University which supplies part of the bibliography.

Status: Report on the heat capacities of the alkali metals will be issued by NBS in FY1966.

Future Plans: Compilation of data will continue. The next publication anticipated will cover the alkaline earth metals and this will be followed by the alkali and alkaline earth oxides. Plans then call for some selected organic data.

B. Compilation Centers Supported by Other Agencies

1. "JANAF Tables" (Joint Army-Navy-Air Force). Preparation of the so-called "JANAF Tables" is conducted as part of a largely experimental program initiated by ARPA, and now supported by the Air Force. The experimental program is carried on at several laboratories which report their results individually. The JANAF Tables are a compilation effort and include data from all sources. The program consists of two parts, one classified and the other unclassified. The effort is confined to the light elements (first two periods of the periodic tables) plus some selected heavy elements; approximately 1/4 of the elements in the periodic table are covered.

Principal Investigator: D. Stull, Dow Chemical Company

Properties Covered: Standard thermodynamic functions as a function of temperature, Heat capacity, Entropy, Gibbs energy (standard and as a function of temperature), Heat of Formation (standard and as a function of temperature); Standard State is 298°K.

Product: JANAF Tables issued quarterly. Two types of tables are issued, white and grey. The white tables contain critically evaluated data, the grey do not.

Status: Tables are constantly being revised and continue to be issued. The Clearinghouse for Federal Scientific and Technical Information (NBS) has recently announced the availability of the existing collection of tables.

Future Plans: Group will continue to exist indefinitely producing tables on a quarterly basis.

2. Light Element Program: This is another part of the ARPA program referred to above. The major activity of the group is experimental; however, approximately two man-years of effort each year are devoted to compilation and critical evaluation of the data produced under the experimental program.

Principal Investigator: C. Beckett, G. Furukawa, and G. Armstrong, National Bureau of Standards.

Properties Covered: Same as 1 above except that standard state is 0°K.

Product: Results appear as semiannual report and go into a general distribution list. The experimental data are incorporated, as appropriate, in the JANAF Tables.

Future Plans: Program is expected to continue along present lines.

Funding: Entirely by DoD.

3. Thermodynamic Data Compilations: The title of the project does not give an accurate description of its activities. The group produces a variety of data compilations; however, the major contribution at the present time is Heat Capacity Data. The project was originally under the direction of K. K. Kelley of the Bureau of Mines, who has now retired.

Principal Investigator: E. King, Bureau of Mines Station, University of California, Berkeley, California

Properties Covered: Heat capacities as a function of temperature from about 20°K. to highest temperature determined.

Product: Tables of Heat Capacity Data

4. Thermal Functions of Rare Earth Elements and Compounds: This project has been recently initiated. It is concerned with the gaseous state from 298°K upwards.

Principal Investigator: R. Feber and C. C. Herrick, University of California, Los Alamos Scientific Laboratory.

Properties Covered: Standard Thermodynamic Functions as a function of temperature, Standard Heat capacity, Entropy, Gibbs energy, Heat of Formation (Standard State 298°K), and Gibbs energy entropy and heat of formation as a function of temperature, and bond association energies.

Product: Ideal gas thermodynamic functions of lanthanide and actinide elements and compounds.

Status: One report has been issued in the Ideal Gas Thermodynamic functions of the elements. A second report on diatomic molecules is in preparation and will be available this calendar year.

Future Plans: The group intends to continue compiling data and publish tables as they become completed.

ORGANIC COMPOUNDS

Compilation activity in organic compounds is limited. There exists a large body of information which should be collected, critically evaluated, and put into a single compilation. The compilation activities which now exist are spotty and do not adequately fulfill the needs identified by panels of consultants. For example, the revision of Parks and Huffman's Free Energies of Some Organic Compounds, which is being done by E. Westrum, D. Stull, and G. Sinke, is scheduled for publication some time in 1966. This project will probably not be kept current.

A. Compilation Activities Supported Entirely by NBS-OSRD

1. Standard Heats of Formation of Organic Compounds: A selected compilation of the standard heats of formation of organic compounds.

Principal Investigator: I. Halow, National Bureau of Standards.

Properties Covered: H_f°

Status: Data have been collected and critical evaluation is proceeding. It is anticipated that a product will be issued in calendar year 1966.

Future Plans: Efforts are being made to increase the level of activity.

B. Compilation Activities Supported by Other Agencies Either Alone or in Cooperation with OSRD

1. Selected Values of Properties of Organic Compounds: This project consists of two parts, the API #44 and the Manufacturing Chemists Association project which is jointly supported with OSRD. API #44 is supported entirely by the American Petroleum Institute and is confined to compilation of thermodynamic and physical properties of hydrocarbons, carbon-hydrogen-sulfur compounds, and carbon-hydrogen-nitrogen compounds. The MCA project is supported jointly by the Manufacturing Chemists Association and NBS-OSRD. Compilation is the same as above but confined to a selected list of compounds decided upon by the technical advisory committee to the MCA project, (primarily oxygen compounds).

Principal Investigator: B. Zwolinski, R. C. Wilhoit, Texas A & M University, College Station, Texas.

Properties Covered: Boiling Point, Freezing Point, density, refractive index, Infra-Red, Ultra-Violet, Nuclear Magnetic Resonance, Mass Spectra, Raman Spectra, Vapor Pressures, and all standard thermodynamic functions.

Product: API and MCA Tables of "Selected Values of Physical and Thermodynamic Properties" issued semiannually (looseleaf) by Texas A & M Press.

Status: Expected to continue indefinitely. Increased level of effort is needed.

Future Plans: Through the cooperation of the MCA advisory panel, the API and the NBS-OSRD it is hoped that this project can be expanded.

Users: The data sheets are sent to more than 1500 organizations (industry and universities).

2. Thermodynamic Properties of Compounds of Biochemical Interest: This is a project funded by NASA.

Principal Investigator: G. Armstrong, National Bureau of Standards

Properties Covered: All standard thermodynamic functions and thermal functions on selected compounds of biochemical interest.

Product: Four quarterly progress reports containing data, as obtained.

Status: Project has been continued on a year to year basis. There is no long term commitment.

Future Plans: All data produced in quarterly reports are to be summarized in one report when sufficient data have been accrued to warrant this.

CRYOGENICS

Under this general heading are grouped those compilation centers that are concerned with the thermodynamic and physical properties of substances at low temperatures. There are no projects in this category supported by NBS-OSRD.

1. Cryogenic Data Center: This is a data center at NBS-Boulder that owes its origin to the liquid hydrogen program at Boulder. This group is now funded entirely by NASA.

The program areas in the Data Compilation Unit are: (1) properties of fluids, (2) properties of fluid mixtures, (3) properties of metallic elements, selected alloys and dielectrics, and (4) mechanical properties of structural materials. At the present time, the Unit's activities are concentrated primarily in the area of properties of fluids. The other program areas will become active as work is completed in the programs for properties of fluids.

Principal Investigator: R. Stewart, V. Johnson, National Bureau of Standards, Boulder, Colorado.

Properties Covered:

(a) All thermodynamic functions
(b) Thermal functions
(c) Vapor pressure data
(d) PVT data on pure substances and mixtures
(e) Physical properties at crogenic temperatures
    1. Dielectric constant
    2. Emissivity
    3. Specific heat
    4. Density
    5. Thermal conductivity
    6. Viscosity
    7. Thermal diffusivity
    8. Surface tension
    9. Electrical resistivity

Status: This is a continuing project supported by NASA and is probably the largest cryogenic data center in existence. The group is undergoing a small expansion and hopes to increase their data compilation capabilities and answering service.

Product: The products are data compilations and bibliographies. Examples of the product are:

(1) The dielectric constant of solid, liquid, and gaseous He, H_2, Ne, N_2, O_2, air, CO, F_2, A, and CH_4.

(2) A bibliography on the thermophysical properties of argon.

(3) Thermodynamic properties of liquid and gaseous argon from 86 to 300°K, with pressures to 1000 atm.

(4) Thermodynamic properties of liquid and gaseous neon from 25° to 300°K, with pressures from 0.1 to 200 atm.

(5) Property differences of ortho and para hydrogen.

(6) A vapor pressure equation for oxygen.

In the next few months, it is anticipated that the following compilations will be issued:

(7) Thermodynamic properties of liquid and gaseous oxygen from 55° to 300°K, with pressures to 200 atm.

(8) Viscosity and thermal conductivity of dilute argon.

(9) Viscosity and thermal conductivity of oxygen.

(10) Viscosity and thermal conductivity of nitrogen.

Future Plans: The group intends to expand their low temperature bibliography in depth to ensure that they are at better than 95% coverage. The answering service will be expanded.

2. Thermodynamic Properties of Helium and Helium Systems: This is a new compilation activity that has been initiated by Bureau of Mines personnel at the Helium Research Center. It will not be competitive with the NBS effort but will supplement it. Excellent cooperation between the two groups exists.

Principal Investigator: L. W. Brandt, Bureau of Mines Station, Amarillo, Texas.

Product: Research information plus compilations of critically evaluated data.

Properties Covered: Probably all thermodynamic and physical properties of the systems (Binary, Ternary, and higher).

Status: Project has only recently been initiated.

PVT RELATIONS

There is considerable activity in this area but usually of a single venture nature. There is as yet no data center that is doing a thorough search of the literature and compiling all existing PVT data.

A. Compilation Programs Sponsored Solely by NBS-OSRD

1. Thermodynamic Properties of Gases Including Polar Gases: This program consists of two parts (1) Thermal properties of gases and (2) Polar gas properties.

Principal Investigator: J. Hilsenrath, National Bureau of Standards

Properties Covered: P-V-T and derived data, and thermodynamic and thermal functions. Theoretical models will be developed which can be fitted to existing data and will provide smooth extrapolation outside of the experimental range.

Product: Part (a) will be essentially a revision of NBS Circular 564. The thermodynamic properties of air from room temperature to 15,000°K will be issued in FY1966. Part (b) will consist of a series of monographs, the first of which will be that on NH_3.

Status: Continuing project. When NH_3 is completed, properties of HF will be obtained. NBS Circular 564 will be revised.

Future Plans: Continue compilation of polar gas properties.

2. Theoretical Studies on Equation of State: The thermodynamic advisory panel has repeatedly emphasized the desirability of supporting theoretical studies on equations of state.

Principal Investigator: S. Y. Larsen, National Bureau of Standards.

Properties Covered: Virial coefficients, Lennard-Jones potentials, P-V-T properties.

Status: The group publishes in the open literature and is very active.

B. Compilation Programs Sponsored by Other Agencies Solely or in Cooperation with NBS-OSRD

1. P-V-T relationships in hydrocarbons.

Principal Investigator: D. Douslin, Bureau of Mines, Bartlesville, Oklahoma

Properties Covered: P-V-T and derived quantities, Cp, density, virial coefficients, Lennard-Jones potentials on pure compounds and mixtures.

Product: Group has been publishing compilations of data as Bureau of Mines bulletins; however, there has been no extensive compilation of PVT data published.

Status: Large scale systematic compilation activities were only recently initiated.

Future Plans: It is the intention of the OSRD in cooperation with the Bureau of Mines to make this one of the largest single centers for the compilation of PVT properties in homogeneous and heterogeneous systems.

SOLUTIONS

The thermodynamics of solutions may be roughly divided into two areas: (1) Electrochemistry and (2) Pressure--Temperature composition relations. In area (1) there is considerable activity, largely because of the urgent needs for these kinds of data. NBS-OSRD is placing considerable emphasis on this area. The product here is mostly in the form of text books.

1. Electrochemistry of Aqueous, Non-Aqueous and Fused Salt Systems. That part of the program dealing with fused salts is discussed under that heading.

A. Aqueous Systems

Principal Investigator: W. Hamer, National Bureau of Standards

Properties Covered: Standard Emf, activities, activity coefficient, conductivities, heats of solution, transference numbers, ionic mobilities.

Status: Literature is being searched and tables of data are being compiled. Two preliminary reports have been issued. Quarterly Report #1 contains statement of conventions, constants, etc. Quarterly Report #2 contains theoretical calculations of activity coefficients. Tables on conductivities are now being prepared. This will be followed by tables of Standard Emf.

Future Plans: Group will continue to compile data and maintain data file on a current status.

B. Non-Aqueous Systems

Principal Investigator: Loren Hepler, Carnegie Institute

Properties Covered: Standard Emf, activities, activity coefficient, conductivities, heats of solution, transference numbers, ionic mobilities.

Status: Literature is being collected and will then be reviewed. This effort is to be coordinated with that above and all conventions, symbols, etc. will be uniform.

Future Plans: Group will continue data compilation and maintain data file on a current basis.

PHASE RELATIONS

The compilation of phase diagrams by various groups throughout the U.S. is quite extensive. If the current level of effort can be increased modestly, coverage for solid systems will probably be adequate. A new activity needed in this area is for liquid-liquid equilibria.

A. Activities Funded by NBS-OSRD

1. Compilation of Binary Metallic Oxide Phase Diagrams: This is a compilation of phase equilibrium relations of 1711 binary metal oxide systems, and is a part of the general activity of a larger group participating in the production of the compilation of phase diagrams for ceramists.

Principal Investigator: R. S. Roth, National Bureau of Standards

Properties: Phase diagrams of binary oxide systems. Melting points of metal-oxides and binary compounds of metal oxides.

Product: NBS Monograph 68 "Melting Points of Metal Oxides" has been issued.

Status: Literature search is completed and critical evaluation proceeding. Diagrams will be available for publication in FY66.

Future Plans: To continue the collection of all pertinent published data referring to the phase equilibrium relations in binary oxide systems and to critically analyze the data.

B. Compilations Funded by Other Agencies Solely Or In Cooperation With OSRD

1. Binary Metal and Metalloid Phase Diagrams: This program is essentially a revision and updating of Hansen's book Constitution of Binary Alloys. The revision is in the form of a supplement, not a completely revised text.

Principal Investigator: R. Elliott, Department of Metallurgy, Illinois Institute of Technology Research Institute (now at the University of Cincinnati).

Properties Covered: Phase diagrams of metal and metalloid systems.

Product: A supplement to Hansen's book, which brings all the data on binary systems up to date, has been published this fall by McGraw-Hill. Next product covering ternary and higher systems is due in approximately two years.

2. Phase Diagrams for Ceramists: This is a program sponsored by the American Ceramic Society. The most recent publication is a compilation of about 2000 phase diagrams.

Principal Investigators: E. M. Levin, C. R. Robbins and H. F. McMurdie, National Bureau of Standards.

Properties Covered: Binary, Ternary, and higher phase diagrams on salts and oxides of the compounds of general interest to ceramists.

Product: Phase Diagrams for Ceramists, American Ceramic Society, Columbus, Ohio, 1964.

Status: New Edition is planned for calendar year 1967 or 1968.

3. Phase Relations of Groups I and II Halides: This is a compilation of about 300 phase diagrams of groups I and II halides.

Principal Investigator: W. D. Robertson, Yale University, Department of Metallurgy

Properties Covered: Binary, Ternary and higher phase relation of groups I and II halides.

Product: Compilation of phase diagrams. Publication plans are uncertain at present.

METALS

A plan is being formulated for a broad interdisciplinary program in the compilation of data pertinent to metals and metal systems. As presently envisioned, the plan calls for the establishment of a coordinating group in the Metallurgy Division at the National Bureau of Standards that will collate data on metals (crystallographic, thermodynamic, metallurgical, mechanical, solid state and chemical) to develop a sort of encyclopedia. The details of this project and the exact nature of the product to be produced remain to be worked out.

A. Projects Supported by OSRD

1. Thermodynamic Properties of Liquid Metals and Liquid Oxides: The program is directed to the critical compilation of the thermodynamic properties of elements dissolved in liquid metals which have been reported

in the literature. An up-to-date, critically compiled tabulation of such data is of fundamental value in the technologies of the extraction and refining of metals. Two of the most important examples are the production of crude steel and the production, or recovery, of uranium. The data are also important to the proper use of liquid metals in heat exchange systems. In addition, the information is important to the scientist who is seeking a basic understanding of the behavior and properties of liquid metals.

Principal Investigator: J. F. Elliott, Massachusetts Institute of Technology

Properties Covered: Activities, activity coefficients, phase relations, solubilities, partial molar quantities.

Product: No product as yet. A contract was initiated in July 1965. Product when issued will be a tabulation of critically evaluated data.

Status: Bibliography is being compiled and data extracted from pertinent papers. First data sheets to be available in July 1966.

Future Plans: This is a continuing project; literature revue and data compilation will continue.

B. Projects Supported by Other Agencies

1. Thermodynamic Properties of Metals and Alloys: This group compiles data on all substances that conduct electricity electronically. Metals and other alloys comprise the bulk of the data.

Principal Investigator: R. R. Hultgran, Department of Mineral Technology, University of California, Berkeley, and part-time assistance of K. K. Kelley also of the University of California.

Properties Covered: All standard thermodynamic functions, thermal functions, vapor pressures, B. P., M. P., activities, activity coefficients, partial molar quantities.

Product: Selected Values of Thermodynamic Properties of Metals and Alloys, John Wiley, 1963. This text is currently being revised. Group also produces data sheets when appropriate and distributes them free of charge.

Status: This project is funded by the AEC and is a continuing project.

FUSED SALTS

A vast body of information exists in this field; however, there has been only limited compilation activity. The Air Force has supported some work, which though reasonably comprehensive, would probably not be regarded as standard reference data. The OSRD is attempting to formulate an overall compilation program in this area.

1. Conductivities in Fused Salt Systems: This work is integrated with the program of Hamer at the National Bureau of Standards for the compilation of conductivities (and other properties) in aqueous, non-aqueous, and fused salt systems.

Principal Investigator: G. Janz, Rensselaer Polytechnic Institute

Properties Covered: Ionic conductivities

Product: Dr. Janz has already issued a preliminary document on the thermodynamic and physical properties of fused salt systems. After further evaluation, a compilation of critically evaluated conductivity data will be issued.

Status: Literature is being reviewed and data evaluated.

Future Plans: This will be a continuing project and the literature search will be maintained current.

2. Thermal Behavior of Inorganic Salts: This project is concerned with data for the thermodynamic properties of fused salts from room temperature up to the highest temperatures recorded for the different salts. The data permit one to calculate the equilibrium constant for the decomposition of the salt at different temperatures.

Principal Investigator: K. Stern, National Bureau of Standards

Properties Covered: Equilibrium constant for the decomposition of all products as a function of temp; Gibbs energy of formation for parent molecules and products, decomposition pressures, densities, melting points, chemical reactions involved in the decomposition, boiling point and some kinetic data.

Product: No product has been issued to date. The salts will be classified according to the anion (sulfates, carbonates, etc.). A compilation on the sulfates will appear in FY66. All data have been coordinated with the revisions to appear in the NBS volume on selected values of thermodynamic properties. (Circular 500 Revised).

Status: A compilation covering sulfates has been completed and will be published within the next four months.

Future Plans: Data on the carbonates will be compiled next, followed by the halides.

TRANSPORT PROPERTIES

A number of projects on diffusion behavior and conductivities have already been mentioned in other categories. For program management purposes it is considered relatively unimportant in which category any specific project is to be listed. The important matter is to be sure that the property is not overlooked because of the assumption it is covered elsewhere.

1. Thermophysical Properties Research Center: This is unquestionably the largest data center in the area of transport properties. The group is housed in its own building constructed by Purdue University for this specific purpose. Until this year the activities of this group have been confined primarily to data compilation and preparation of bibliography. However, the group is now in the process of establishing extensive research capabilities. One of the important services any large well organized data group can perform is to provide bibliography, and reprints of papers.

Principal Investigator: Y. S. Touloukian, Purdue University

Properties Covered: Thermal conductivity, specific heat, viscosity, fluidity, emissivity, absorptivity, reflectivity, transmissivity (total and spectral) diffusion coefficients, permeability, thermal diffusivity, Prandtl number, surface tension, and density of solids.

Product: Retrieval Guide, compilation of critically evaluated data on thermal conductivity of solids, liquids, gases. Bibliographies upon request; question and answering service. Critical data compilation activity emphasizes thermal conductivities. This will be expanded shortly.

Status: Continuing project funded largely by DOD, but has substantial support from OSRD. The program also has limited support from other agencies.

Future Plans: Compilation capabilities on emmisivity are now being developed. With the aid of Dr. Mikato of Kyota University, compilation on selected heat capacities have been initiated which will permit some compilation capability on Prandtl numbers.

VII. CHEMICAL KINETICS

Compilation, evaluation and tabulation of numerical data in the field of chemical kinetics presents a number of individual problems. By definition, the system is changing in composition; the reaction mechanisms may be uncertain, or may change with temperature or other parameters; catalysts, wall-effects and other local influences may be significant. Previous attempts to present kinetic data in tabular form (e.g., NBS Circular 510, Tables of Chemical Kinetics - Homogeneous Reactions, with two supplements, prepared under the direction of N. Thon and Charles Stauffer) have found the difficulties substantial.

The NAS-NRC Committee on the Kinetics of Chemical Reactions agreed to act as the Advisory Panel to the National Standard Reference Data System for Chemical Kinetics, and met in this capacity in January, 1964.

In summary, the Committee recognized the difficulties inherent in any undertaking to evaluate and compile in tabular form the large amount of numerical data to be found in the literature on rates of chemical reaction. Unlike the field of thermodynamics where it is possible to reduce data to an internally consistent body of well-defined quantities, the experimental parameters of chemical kinetics do not lend themselves to such unification. Insufficient understanding of the effects of the many variables which must be specified in the description of a single experiment preclude establishment of categoric rules for the presentation of chemical kinetic data in all but relatively few cases.

The committee recommended that the best approach to the compiling of the data would be to divide chemical kinetics into areas and to assign each area to a qualified specialist. Each would prepare a critical review of the area, with emphasis on the quantitative aspects of that field. These reviews would be published as a series of monographs. A list of approximately forty recognized specialists in the various fields of chemical kinetics was prepared. The Chairman of the Committee agreed to develop a staff of scientists interested, willing and available to undertake the reviews and preparation of monographs. Availability of funds will require establishment of priorities of topics to be undertaken, and the Committee accepted the responsibility to review the proposals and recommend a priority schedule. Initial proposals would be submitted to the Office of Standard Reference Data, National Bureau of Standards for preliminary screening and then forwarded to the Committee for its review. Because of the philosophy of separate specialized critical review monographs, the Committee preferred not to develop a comprehensive list of properties, or a definition of the field.

The recommendations of the Committee have been followed by NBS staff members in the OSRD and in the Division of Physical Chemistry. A substantial number of proposals for monographs on specific topics have been submitted by highly qualified scientists. The projects are being supported by contracts to the extent that funds are available.

The ensuing is a list of projects now being activated:

1. Title of Project: Chemical Kinetics Information Center

   Principal Investigator: David Garvin, Physical Chemistry Division, NBS
   Washington, D.C.

Technical Scope and Plan of Operation: The Center consists of articles in the general field of chemical kinetics which are entered into a file with an inverted index arranged according to various descriptive terms as well as by author, chemical compound, bibliographic reference and institution. The file can be searched by selection of appropriate descriptive terms. The purpose of the Center is to provide an extensive, and perhaps, eventual comprehensive collection of literature for use in the production of critical reviews of data in the kinetics field, and for other uses which might require the availability of such an extensive collection. The indexing system is expected to provide speed and flexibility in bibliographic searching over conventional storage and indexing rechniques. The services of the Center will be offered to all contractors of the NSRDS who are preparing critical reviews in the kinetics field.

This Center is jointly supported by the Department of Defense Advanced Research Projects Agency and by NBS-OSRD.

Current Status: Operational. The Center is in an early operational phase and has not yet acquired sufficient entries to have reached full operational status.

Products Issued or to be Issued: None contemplated at the present time.

Future Plans: Efforts will be made to bring the Center, as soon as possible, to a suitable size that meaningful tests can be made of the effectiveness and speed of the indexing system. Assistance will be offered to all contractors for critical reviews as their projects become operational.

2. Title of Project: Radiation Chemistry Data Center

Principal Investigator: Milton Burton, Radiation Laboratory, Notre Dame

Technical Scope and Plan of Operation: The main objective of the Radiation Chemistry Data Center is compilation of kinetic data from reactions induced by ionizing radiation on chemical systems. The data may be in the form of specific rates of elementary processes or overall reactions; radiation chemical yields (G) reported in molecules of product (or intermediate) per 100 ev.; effects on physical properties, such as electrical resistance, viscosity, etc. Evaluation and interpretation of such data will be done by experts in each of the pertinent branches of radiation chemistry.

A selected group of journals (including Chemical Abstracts and Nuclear Science Abstracts) is scanned regularly; each reference of interest is recorded on a worksheet along with descriptors which classify the information. The molecular formulas of reactants, products and intermediates are recorded on data sheets, which will include a description of the chemical system, irradiation conditions, and the data reported.

The descriptors and molecular formulas will be stored by a suitable system. Retrieval will provide bibliographic information to answer inquiries and as an aid to preparing summaries of information and compilations of data for critical review.

This project is supported jointly by the Atomic Energy Commission and OSRD. AEC also supports associated experimental and theoretical research programs at this location.

Current Status: The current literature is being covered by postdoctoral research associates along with the Radiation Chemistry Data Center staff. A list of descriptors is to be developed. Work has begun on a compilation of specific rates of processes in aqueous systems (e.g., reactions of the hydrated electron, hydrogen atom or hydroxyl radical with various solutes). Papers not covering this subject are being stock-piled for indexing and for later recording of the data therein.

Products Issued or to be Issued: It is hoped to issue a critical review of specific rates in aqueous systems in about a year. Publication plans will be made with recognition of the joint support of the project by AEC and OSRD.

Future Plans: Current papers on radiation chemistry will be indexed and reader-compilers will record the data for compilation and critical review purposes. Arrangements are planned for investigators in other countries to cover the literature in their native languages.

3. Title of Project: Heavy Isotope Effects

Principal Investigator: Marvin J. Stern, Yeshiva University, New York City
Max Wolfsberg, Brookhaven National Laboratory
Jacob Biegeleisen, Brookhaven National Laboratory

Technical Scope: The monograph will contain:

(1) A discussion of the theory of kinetic isotope effects. This discussion will be applicable to hydrogen isotope effects as well as to heavy-atom isotope effects although items of theory concerned almost exclusively with hydrogen effects (e.g., quantum mechanical tunneling) will be discussed very briefly.

(2) A discussion of experimental aspects of isotope effect studies.

(3) A tabulation and critical review of experimental work (including theoretical interpretation) of heavy-atom kinetic isotope effects in *in vitro* chemical reactions.

The following "fringe" subjects will not be included.

(1) Isotopic geochemistry (except for pure chemical studies included in geochemistry papers).

(2) Isotope effects in living systems.

(3) Isotope effects in mass spectrometry and other electron-impact processes.

(4) Isotope effects in electrochemical processes.

(5) Isotope effects in processes not involving chemical change (except for rates of precipitation reactions).

(6) Isotope effects in radiation and hot-atom chemistry.

(7) Isotope effects due to selective excitation of isotopes rather

than on the reaction process itself.

(8) Isotope effects in diffusion-controlled processes.

The approach to these topics will emphasize both the general scientific interest and the specific concern of atomic energy research scientists. Such emphasis is especially appropriate in view of the joint support of the project by AEC and OSRD.

Products to be Issued: The monograph being prepared will be issued through NBS, probably as one of the NSRDS-NBS series. Additional distribution through the Atomic Energy Commission channels will be considered.

Current Status: The literature search for articles related to a critical review monograph on heavy-atom isotope effects is now complete through late 1964. Final completion must await the publication of the June, 1965, index to Chemical Abstracts. Approximately 600 pertinent articles have been collected and cataloged. Extraction of information from these articles is now underway.

Future Plans: The following recommendations regarding the inclusion of items 1-8 above in future monographs are made, with the recognition that they should be covered in later projects:

Items 1 and 2 should be included in separate monographs, although it is questionable if such monographs belong in a kinetics series. Items 3 and 4 together should be the subject of a separate monograph. Items 5, 6, and 8 should be included in monographs covering the general subjects. Item 7 should probably be included in a monograph on isotope separation and enrichment (not part of a kinetics series).

The extensive subject of hydrogen kinetic isotope effects can conveniently be subdivided as follows:

1. Primary hydrogen isotope effects
2. Secondary hydrogen isotope effects
3. Solvent hydrogen isotope effects.

4. Title of Project: A Critical Monograph on Quantitative Kinetic Data in the Field of Unimolecular Reactions

Principal Investigator: Sidney W. Benson, Stanford Research Institute

Technical Scope and Plan of Operation: Plans are to summarize and review all of the kinetic data on unimolecular, gas phase reactions available in the scientific literature up to and including 1 November 1965. The data will be critically examined to estimate reliability of the work and limits of error on the rate constants and their Arrhenius parameters, i.e., the temperature dependence of the rate constant. Also to be examined are data from the point of view of self-consistancy by using thermochemical data and data on the inverse association reactions.

Current Status: The project is still in the stage of compilation of data and establishing ground rules for categorizing and describing it. This phase of the work is nearly completed.

Products Issued or to be Issued: None yet. Final product will be a detailed critical review. Publication arrangements are not yet settled.

5. Title of Project: Tables of Kinetics of Homogeneous Gas Reactions

Principal Investigator: A. F. Trotman-Dickinson, Edward Davis Chemical Laboratory, Aberystwyth, U.K.

Technical Scope: This monograph is concerned with the preparation of complete critical tables of data on the kinetics of all gas reactions for which suitable information is available. Many gas reactions do not occur simply as they are written in a conventional chemical formula. They take place in a series of steps known as elementary reactions. The same elementary reactions may be common to a large number of different reaction systems. Because of their fundamental nature, elementary reactions will be the concern of the tables, and will be the basis for the tabular portion of it. The text will also contain critical assessment and commentary on the numerical data.

Products Issued or to be Issued: This monograph will be issued as a report in the NSRDS-NBS series.

Current Status: A card index has been prepared of some 2,000 references culled from reviews. This bibliography forms the basis for the critical assessment.

Future Plans: A comprehensive survey and selection of the appropriate data on elementary reactions and the tabulation of the data is now underway. It is expected that the review will be complete by the end of the summer of 1966.

6. Title of Project: Solvent Effects in Solution Kinetics

Principal Investigator: G. C. Akerlof, Princeton, New Jersey

Technical Scope: A selected compilation of tabular data is being prepared on the topic of solvent effects in solution kinetics, with particular attention to organic solvent systems. A complete bibliographic survey has been prepared and selected tables extracted from the references. Accompanying the numerical information will be a synopsis and summary of the state of quantitative knowledge in each of the specific subtopics covered by the review, with appropriate commentary on limitations of applicability of the numerical data.

Products Issued: The compilation and bibliography will probably be issued through NBS and GPO channels.

Current Status: More than 5,000 references have been studied and tables of the most reliable data have been extracted therefrom. A draft manuscript is being prepared, and with the exhaustive bibliography there will be probably over 1,000 pages of material.

Future Plans: The literature on solution kinetics is very extensive, and the monograph will contain a great deal of quantitative information. Since the volume of data is so large, it may prove desirable to have additional critical analysis made of certain subtopics within this field. If so, the present monograph will form a valuable starting place.

7. Title of Project: Bibliography of Small Molecules Gas Phase Reactions

Principal Investigator: A. Hochstim, Institute for Defense Analyses
Washington, D.C.

Technical Scope: This project is not a part of the series of critical review monographs described above, nor is it directly supported by the National Standard Reference Data System. It was the purpose of this work to provide a comprehensive bibliography of gas phase reactions of atoms, and molecules, containing not more than five atoms, as a basis for further analysis and critical review. The work was supported by the Department of Defense Advanced Research Projects Agency under contract with the Institute for Defense Analysis. Since the work is bibliographic rather than critical in nature, the technical scope is limited to a careful itemization of the reaction, the reaction conditions and appropriate reference material.

Products to be Issued: This bibliography is based on more than 6,000 references and contains over 10,000 index items. It will be issued as a reproduction of computer tape printout. It may also be available in the form of duplicates of the computer tape.

Current Status: The computer tape is now being checked for errors and the errors are being corrected. Publication is scheduled for mid 1966.

Future Plans: The sponsor of this project, the Advanced Research Projects Agency, has arranged to have this bibliographic collection taken over and maintained by the Chemical Kinetics Information Center at the National Bureau of Standards, and is supplying funds to NBS for this purpose. It will be used as source material for authors of critical review monographs in the Chemical Kinetics series.

SUPPLEMENT TO STATUS REPORT, NSRDS

CHEMICAL KINETICS CONTRACTS

8. Title of Project: Hydrogenation of Ethylene on Metallic Catalysts

Principal Investigator: Juro Horiuti, Research Institute for Catalysis, Hokkaido University, Sapporo, Japan

Technical Scope: The hydrogenation of ethylene on metallic catalysts is more thoroughly understood than almost any other gas phase reaction involving a solid catalyst. Both on the basis of theory and with regard to the sophistication of experimental measurements, this system is a prototype for data compilation activities in this general area. The principal investigator will present all available "raw data"on the hydrogenation process by diagrams insofar as the accuracy of the primary data is thus sufficiently reproduced. This will include, besides the rate of the hydrogenation itself as a function of partial pressures and temperatures, the rates of parahydrogen conversion, H_2, D_2-equilibration and formation of different deuteroethylenes and deuteroethanes respectively associated with the hydrogenation in question, inclusive of deuteration and the reproducibility of these rate measurements. Second, he will critically review these observations with regard especially to the reproducibility; the usual procedure of referring the observed rate at a specified condition to that subsequently determined at a "standard" condition to reduce the poisoned rate to unpoisoned one is not secured, since the poison may affect the rate law as well. Third, he will present the mechanisms hitherto proposed and decide mechanism or mechanisms which fits in with the experimental results critically warranted in the second step mentioned above.

It is recognized that, even with these precautions the subject of this monograph presents serious problems regarding its suitability for providing Standard Reference Data. The decision to support this project was made after obtaining advice on its potential usefulness from representatives of academic and industrial scientists who are concerned with this field.

Products Issued or to be Issued: This monograph will be issued as a report in the NSRDS-NBS Series.

Current Status: This project was authorized in November of 1965. The survey is in its initial stages at present and full work will not start until the summer of 1966.

Future Plans: When this monograph has been completed it will be studied in the determination of plans in the selection of other projects in the review monograph series.

Supplement to Status Report, NSRDS (Cont'd)

Chemical Kinetics Contracts

9. Title of Project: The Reactions of Nitrogen, Oxygen and Oxides of Nitrogen.

Principal Investigator: Prof. Harold S. Johnston, University of California, Berkeley, Calif.

Technical Scope: The principal investigator will prepare a critical review of all the reactions involving nitrogen and oxygen of five atoms or less, with emphasis on neutral species. In making the review, he will draw on the bibliographic resources of the Chemical Kinetics Data Center at the NBS, which will provide him with access to the bibliography of small molecule gas phase reactions, prepared under the direction of Dr. A. Hochstim of the Institute of Defense Analyses.

Products Issued or to be Issued: Since this project is being supported by NBS with funds made available from the Advanced Research Projects Agency, the principal investigator will prepare a preliminary report summarizing in a general way the state of quantitative knowledge in the subject indicated without detailed attention to a critical analysis of the data themselves. In addition he will provide a final report and bibliography which will be issued as part of the NSRDS-NBS Series.

Current Status: Active work on this project is expected to begin in April 1966 and should be completed by October 1966.

Future Plans: The principal investigator has indicated that following the completion of the present volume, he will use his experience gained in the first stages of the work to determine the desirability of extending the coverage to include molecules of more than five atoms. This project would be supported separately.

10. Title of Project: Elementary Reactions of the Hydroxyl Radical.

Principal Investigator: Prof. Leon K. Dorfman, Ohio State University, Columbus, Ohio

Technical Scope: Modern investigative techniques, including electron spin resonance spectroscopy and pulse radiolysis are capable of generating reliable data on hydroxyl reactions in sufficient quantity to justify a critical review of all such reactions. Reactions will be reviewed according to the following classification system:

1. Organic addition reactions
2. Hydrogen abstraction reactions
3. Charge transfer reactions
4. Radical-radical reactions
5. Reactions of O

Special attention will be given to the following points:

1. Critical appraisal of the reliability of the identity of the elementary reactions.

2. Careful evaluation of the level of confidence of the numerical values for each rate constant.

3. Clear-cut distinction between absolute and relative rate constants.

Products Issued or to be Issued: The compilation and bibliography will be issued as a monograph in the NSRDS-NBS Series.

Current Status: Work on this project has not yet begun. It is estimated that the formal compilation and writing would be started in 1966 and completed in 1967.

VIII. COLLOID and SURFACE PROPERTIES

Late in 1961 a Committee on Colloid and Surface Chemistry was created within the National Academy of Science--National Research Council. Chairman of this Committee is Dr. A. C. Zettlemoyer, Lehigh University. The Committee is the national analog of the Commission on Colloid and Surface Chemistry of the International Union of Pure and Applied Chemistry. Chairman of this Commission in IUPAC is Sir Eric Rideal, and its Secretary Dr. W. A. Zisman, U. S. Naval Research Laboratory.

In the fall of 1962 a subcommittee of the NAS-NRC Committee was organized to initiate a critical data compilation program in the fields of colloid and surface chemistry. This subcommittee consists of Dr. H. van Olphen, Chairman, and Dr. T. F. Young and Dr. B. Roger Ray, members. The subcommittee was intended to cooperate closely with the Office of Critical Tables of the National Academy of Science, and when the National Standard Reference Data Program was initiated at the National Bureau of Standards, collaboration with the Program was also established. The subcommittee keeps the Office of Standard Reference Data at NBS informed about the progress on the various projects which have been initiated and it makes suggestions for the establishment of contractural arrangements between NBS and data compilation groups whenever needs for financial support exist.

On the basis of the replies to a questionnaire which was circulated among the members of the NAS-NRC Committee and a number of other experts in the U. S. and abroad, the following course of action was decided upon: The rigorous standards adhered to in most of the original Critical Tables were also adopted for the present program. About a dozen topics were selected for further consideration. The selection was primarily guided by the criteria of usefulness of compilations to the scientific and industrial community, and of the availability of significant data in the literature. In the future, the program may be extended to other topics if the need arises.

The actual work was organized as follows: For each topic a well known expert in the particular field was invited to act as project coordinator. He assumes the responsibility for the final compilation. He selects a number of experts to perform the actual compilation work with the assistance of student and nonprofessional help. For reasons of administrative expediency, project coordinators have been selected from groups of scientists residing in the U. S. with one exception. In order to obtain optimum results expert collaborators have been partly selected from the international scientific community for some of the projects. The Chairman of the NAS-NRS subcommittee coordinates the efforts of the various project groups, and maintains the liaison with NSRDS and with the Office of Critical Tables.

A. Colloidal Systems

1. Light Scattering. Clarkson College of Technology has established a critical data center for the purpose of collecting and evaluating data produced in the area of light scattering.

Title of Project: Critical Data Center - Light Scattering

Principal Investigator: Milton Kerker, Clarkson College of Technology, Potsdam, New York

Technical Scope and Plan of Operation: The experimental areas which the Clarkson Center is considering are:

1. Liquids

2. Solutions including macromolecular, polyelectrlyte, miceller, polyanionic, electrolytes, etc. solution. Both internal interference effects due to finite particle size and those interference effects due to ordering of the particles by interparticle interactions will be considered.

3. Colloidal dispersions including both systems prepared in the laboratory as well as naturally occurring dispersions such as clouds, dust, smoke, milk, etc. In addition to the usual interest in particle size effects, attention will also be directed to absorption effects (colored metal sols) and refraction effects.

The computational and theoretical areas which the Clarkson Center is considering are:

1. Boundary value solutions for particles with spherical and cylindrical symmetry.

2. Rayleigh-Gans solutions for various configurations and structures.

The work on computational and theoretical results would consist of listings of published calculations, not the calculations themselves. Also, there would be compilations of useful formulas. A major area of concern will be listings of computer centers having suitable programs available and possibly critical evaluation of programs as well as publications of selected programs. The center would also arrange to produce selected computations upon request.

The center operates by carrying out systematic literature searches in the usual way.

The final products of this center will consist of the following:

1. Tables of data, critically annotated.

2. Critical evaluations of experimental procedures, especially calibration procedures and correction factors.

3. Tables of useful formulas.

4. Selected critical bibliographies, critically annotated.

5. Critical reviews of specialized topics.

6. Computer programs.

7. Listings of published tabulations of theoretical functions.

Current Status: A critical evaluation of Rayleigh Ratios and polarization values of liquids is in progress.

Products Issued or to be Issued: A report of the above work will be issued within the year.

Future Plans: Continuance along lines outlined.

2. Precipitation Kinetics.

Principal Investigator: Victor K. LaMer, Columbia University

Current Status: Not active as yet.

3. Critical Micelle Concentration Data on Association Colloids. A large class of solutions presents the peculiarity that at low concentrations, their behavior is essentially ideal whereas above a relatively sharply defined concentration large colloidal aggregates called micelles are present. This concentration is called the critical micelle concentration.

The critical micelle concentration or cmc is a measure of the balance between the hydrophilic tendencies of the particle which tend to keep it dispersed and the hydrophobic tendencies which tend to hold it at the surface or interface and to make it aggregate into micelles. It can vary greatly with the structure of the compound and can be readily determined by a number of methods, several of them quite widely applicable and reasonably concordant. In practice, the values cover a range of about four decades and can be determined to a percent or so. They are sensitive not only to the structure of the compound but also to the solvent used -- salts, organic additives, cosolvents, impurities -- to the temperature and pressure although the latter is of lesser general importance.

The cmc is therefore used to characterize the compounds as a criterion of their purity and identity, as a guide to their practical applications and as a tool in the study of interparticle forces. It also plays the same role in the study of properties of micelles as infinite dilution plays in the study of polymers since at the cmc the interaction between micelles vanishes although the concentration of the compound is finite.

Thousands of values of cmc for hundreds of compounds are scattered through the literature. Some were obtained in basic physical-chemical studies, others in connection with applications in industry (detergents, polymers, emulsions, paints, petroleum production, pharmaceuticals, etc.) or in science (analysis, biology, pharmacology, kinetics, etc.). Some are precisely and accurately determined on pure compounds and others are less precise or accurate and involve materials of questionable purity and some are only upper or lower limits or may involve commercial mixtures.

Title of Project: Critical Micelle Concentration Data Group

Principal Investigator: Karol J. Mysels, University of Southern California, Los Angeles, Calif.

Technical Scope: To collect the available data, to make them easily accessible for searching from a variety of viewpoints, to evaluate and classify them as to reliability and to make the results readily available to others and easy to keep up to date.

Current Status: In the process of abstracting and evaluating the informa-

tion on hand, and placing it on IBM cards. At the same time we continue to collect the literature as additional references come to our attention.

Future Plans: To complete this stage, to proceed to the selection of evaluated values for final presentation and then to keep the work up to date.

4. Surface Tensions of Solutions of Association Colloids.

Principal Investigator: C. R. Singleterry, U. S. Naval Research Laboratory

Technical Scope: Surface tension data on solutions of association colloids (conventional soaps and synthetic detergents, as well as certain dyes) will be collected. Effects of temperature, and of the presence of a third component (electrolytes) will be considered, as well as the dependence of the surface tension on the concentration. The latter constitutes a method for the determination of the critical micelle concentration (cmc) in these solutions from a discontinuity in the surface tension-concentration curves. Therefore, close contact with the compilation work on cmc data in Dr. K. Mysels' project will be maintained. At the same time there will be coordination with Dr. Young's project on surface tensions of one component systems in order to guarantee uniformity of treatment.

Current Status: In the stage of literature retrieval.

B. Properties of Surfaces and Interfaces

1. Title of Project: Surface Tensions of Liquids, Contact Angles at Interfaces

Principal Investigator: T. Fraser Young, Argonne National Laboratory;
Collaborators: H. M. Feder, Argonne National Laboratory, G. Janz, Rensselaer Polytechnic Institute, J. J. Jasper, Wayne State University

Technical Scope: Essentially the same as that of the group of extensive tables in the original International Critical Tables. (Volume IV, pp. 434-475) The present updating efforts are as follows:

a) Tensile strength and angle of contact.
b) Methods of measuring surface tension.
c) Interfacial tension for solid-liquid and liquid-liquid interfaces.
d) Surface tension of metals.
e) Surface tension and related properties for temperatures below 0°C.
f) Surface tension of fused salts above 200°C and liquids above 360°C.
g) Surface tension data for certain pure liquids between 0 and 360°C and for all types of solutions at all temperatures.

2. Title of Project: Data on Physical Adsorption of Gases on Solids

Principal Investigator: S. Brunauer, Clarkson College of Technology

Current Status: In process of activation.

3. Title of Project: Data on Chemisorption

Principal Investigator: None assigned yet.

Current Status: Discussion session recently held at NBS.

Future Plans: To be activated.

4. Title of Project: Solid-liquid interfaces-heat of wetting.

Principal Investigator: A. C. Zettlemoyer, Lehigh University

Collaborators: Dr. Boucher, Lehigh University
D. W. Fuerstenau, University of California, Berkeley
G. D. Parfitt, University of Nottingham, England
P. A. Pethica, Unilever, England
J. Taylor, Unilever, England

Technical Scope: A modest amount of data on heats of adsorption and of wetting of solids by liquids were compiled in the International Critical Tables by H. R. Kruyt and J. G. Modderman (Volume V, pp. 139-143). Only two pages of this chapter deal with heats of wetting. A comprehensive survey of the literature on heats of wetting data is planned by the present group. The retrieval work is divided between the collaborators on the basis of country of origin of the literature.

Current Status: In the stage of literature retrieval.

5. Title of Project: Electrical Properties of Interfaces.

Principal Investigator: J. Lyklema, Agricultural University of Wageningen, Netherlands

Collaborators: B. H. Bijsterbosch, Wageningen, Netherlands
R. H. Ottewill, Bristol, England
R. H. Parsons, Bristol, England
Prof. A. Watillon, Brussels, Belgium
A. Watanabe, Osaka, Japan
(Russian cooperation is being studied.)

Technical Scope: The project is concerned with the collection and critical evaluation of data on the electrical properties of interfaces (viz: double layer charge, double layer capacity, electrocapillary curves, electrokinetics, surface conductance).

Plan of Operation: First stage: non-critical compilation of literature references that might contain useful data (Screening in width). Second stage: slightly more critical screening of the retrieved literature (Screening in width with more depth). Third stage: final critical evaluation of data (screening in depth). Fourth stage: assembling of the collected critically evaluated data for print. During the course of the work six semi-annual reports will be delivered. The final report can be expected in April 1968.

Current Status: The first stage is now nearly completed. The first semi-annual report is in course of preparation.

Products to be issued and future plans: Second semi-annual report, due April 1966 will contain references with a high degree of completeness and a "grading" as to the quality and/or other relevant properties of the material. The third and following reports will contain only limited amounts of material but with a full critical evaluation. This critical evaluation is expected to

be completed with the sixth semi-annual report, in April 1966.

6. Title of Project: Properties of monolayers on liquid surfaces and interfaces.

Principal Investigator: H. E. Ries, Jr., American Oil Company

Technical Scope: The desired scope is still under discussion. One group of experts feels that in most of the published work purity of the materials used is questionable and that only very few data exist which can stand critical evaluation. They propose to prepare a brief critical review of techniques and sources of uncertainty, together with data on the one or two compounds which can be safely used for calibration purposes of instruments. Another group, however, feels that in spite of this situation, there is much useful information in the literature worth compiling. Such information may consist of pressure-area behavior of monomolecular layers, effect of the substrate, and potential measurements on spread monolayers.

7. Title of Project: Mass Transport through Surface Films.

Principal Investigator: V. K. LaMer, Columbia University

Present Status: Not activated as yet.

IX. MECHANICAL PROPERTIES

In this area there has been a preliminary examination by an internal NBS panel of the important properties to be considered for possible compilation projects. The purpose was to prepare working papers for review and recommendations by a panel of specialists broadly representative of the governmental, industrial, and academic technical communities.

The NBS panel agreed on the need for critically evaluated data on the mechanical properties of materials, although there was also clear recognition of the fact that some areas of the field were not well enough advanced, either theoretically or experimentally, to warrant their inclusion within the present guidelines of the NSRDS.

The question of how far one could or should go toward including engineering materials or engineering type data in the Standard Reference Data Center was discussed. It was concluded that simple categorical statements on this point were out of order. It seems necessary to consider separately each material/property combination which is proposed for inclusion in the Center. The structure of the material must be characterizable explicitly or operationally, by specifying its composition and previous history, sufficiently well so that the value ascribed to the property can be reproduced by another investigator. This factor also implies that the measurement technique is itself easily and significantly characterizable. The reason for considering both the material and the property together before making a decision is that a degree of characterization of a particular substance which is adequate for its elastic properties may be totally inadequate for the specification of many aspects of its plastic behavior. This is true even for a single crystal of a pure element.

In order to consider the whole field of mechanical properties in an orderly manner, a material/property matrix was developed. Members of the committee with special knowledge in the specific fields blocked out in the matrix then gave detailed consideration to the blocks of the matrix and prepared reports describing:

1. The properties of types of data which are of primary importance in the field and which are sufficiently well understood and measureable so that a critical evaluation of the data can be made;

2. The most suitable form for presentation of the data (i.e., tables, graphs, review articles, etc.);

3. Suggestions of individuals who are experts in each field and who might be called on to participate in the program.

Where the methodology of measurement greatly affects the value ascribed to a property, and this is true primarily in the field of plastic behavior, it seemed appropriate to present the data in the form of a review (i.e., the hardness of the solid elements) rather than as tabulated data. It was suggested that the reviews could follow a common format covering at least certain specific properties deemed to be basic. This approach may well be the best way to handle plastic deformation data. When all of the reviews are in, it might then be possible to make up useful and significant tables of data on some specific property for all of the elements.

As a start, one should probably consider only the nominally pure elements. As time goes on, binary systems of particular scientific or technological importance, that is, certain oxides or alloys or simple compounds can then be included. Here, too, however, one needs to bear in mind the material/property combination rather than just the material or the property.

At a convenient date in FY66, it is planned to discuss the above views with an advisory panel on mechanical properties and then to plan an action program, if any is recommended.

APPENDIX A

Advisory Panels of the

Office of Standard Reference Data

I Nuclear Data Projects

Dr. Henry H. Barschall, University of Wisconsin
Dr. E. Richard Cohen, North American Aviation, Inc.
Dr. Joseph L. Fowler, Oak Ridge National Laboratory
Dr. William A. Fowler, California Institute of Technology
Dr. Gertrude S. Goldhaber, Brookhaven National Laboratory
Dr. Harry E. Gove, University of Rochester
Dr. William W. Havens, Columbia University
Dr. H. W. Koch, National Bureau of Standards
Dr. George A. Kolstad, Atomic Energy Commission
Dr. Carl O. Muehlhause, National Bureau of Standards
Dr. I. Perlman, Lawrence Radiation Laboratory
Dr. Richard F. Taschek, Los Alamos Scientific Laboratory
Dr. Ira Zartman, Atomic Energy Commission

II Atomic and Molecular Properties

Dr. W. R. Bennett, Yale University
Dr. L. M. Branscomb, National Bureau of Standards
Dr. E. U. Condon, University of Colorado, Chairman
Dr. Paul Cross, Mellon Institute
Dr. R. H. Garstang, University of Colorado
Dr. L. F. Johnson, Varian Associates
Dr. Aron Kuppermann, University of Illinois
Dr. E. R. Lippincott, University of Maryland
Dr. Allen Lurio, International Business Machines
Dr. D. P. Stevenson, Shell Development Company
Dr. Brian Whyborne, Argonne National Laboratories
Dr. Richard Zare, University of Colorado

III Solid State

Dr. J. H. Crawford, Oak Ridge National Laboratory, Chairman
Dr. Simon Foner, Massachusetts Institute of Technology
Dr. H. P. R. Frederikse, National Bureau of Standards
Dr. Walter Hibbard, General Electric Company
Dr. John Hulm, Westinghouse Electric Corporation
Dr. David Lazarus, University of Illinois
Dr. D. K. Stevens, Atomic Energy Commission
Dr. M. Tanenbaum, Western Electric Company
Dr. Robert Terhune, Ford Motor Company
Dr. David Turnbull, Harvard University
Dr. George Vineyard, Brookhaven National Laboratory
Dr. Ferd Williams, University of Delaware

IV Thermodynamics and Transport Properties

Dr. Charles W. Beckett, National Bureau of Standards
Professor L. N. Canjar, Carnegie Institute of Technology
Dr. R. E. Duff, Lawrence Radiation Laboratory
Dr. Leo Friend, M. W. Kellogg Company
Professor Joseph Kestin, Brown University
Dr. Joseph F. Masi, Air Force Office of Scientific Research
Dr. John P. McCullough, Socony Mobil Oil Company
Dr. Richard A. Oriani, U. S. Steel Corporation
Professor Bruce Sage, California Institute of Technology
Dr. Frederick D. Rossini, University of Notre Dame, Chairman
Dr. Fred Schulman, National Aeronautics Space Administration
Dr. A. R. Van Dyken, Atomic Energy Commission
Dr. Guy Waddington, National Academy of Sciences-National Research Council
Dr. Thomas J. Webb, Merck, Sharpe and Dohme
Professor Edgar F. Westrum, Jr., University of Michigan
Dr. Bruno J. Zwolinski, Texas A & M University

V Chemical Kinetics

Dr. S. H. Bauer, Cornell University
Dr. Jacob Bigeleisen, Brookhaven National Laboratory
Dr. Milton Burton, University of Notre Dame
Dr. Henry Eyring, University of Utah, Chairman
Dr. J. O. Hirschfelder, University of Wisconsin
Dr. Harold S. Johnston, University of California
Dr. Martin Kilpatrick, Argonne National Laboratories
Dr. Richard M. Noyes, University of Oregon
Dr. Charles N. Satterfield, Massachusetts Institute of Technology
Dr. Merrill B. Wallenstein, National Bureau of Standards

VI Colloid and Surface Properties

Dr. Stephen Brunauer, Clarkson College of Technology
Dr. H. Heineman, M. W. Kellogg Company
Dr. Victor K. LaMer, Columbia University
Dr. Franklin S. Long, Cornell University
Dr. H. van Olphen, Shell Development Company
Dr. B. Roger Ray, Washington State College
Dr. T. F. Young, Argonne National Laboratories
Dr. A. C. Zettlemoyer, Lehigh University, Chairman
Dr. William A. Zisman, U. S. Naval Research Laboratory
Mr. Martin Paul, National Academy of Sciences-National Research Council

VII Mechanical Properties

Dr. W. Haller, National Bureau of Standards
Mr. L. K. Irwin, National Bureau of Standards
Dr. L. K. Kushner, National Bureau of Standards
Mr. P. Macedo, National Bureau of Standards
Dr. R. S. Marvin, National Bureau of Standards
Dr. M. R. Meyerson, National Bureau of Standards
Dr. E. Passaglia, National Bureau of Standards
Dr. A. W. Ruff, Jr., National Bureau of Standards
Dr. J. B. Wachtman, National Bureau of Standards

APPENDIX B

Property Lists

IB List of Properties in Nuclear Data

Energy levels
Total angular momentum quantum number
Orbital angular momentum quantum number
Transition probability
Integral conversion coefficient
Particle energy
Beta energy
Gamma energy
Electric quadrupole moment
Magnetic dipole
Magnetic octupole
Reaction energy
Half-life (mean life)
Level width
Nuclear level density
Angular correlation function
Number of neutrons per fission
Parity resonance integral
Cross section: scattering, absorption, total charge particle reaction
Fission product yield

IIB Atomic and Molecular Properties

A. Fundamental constants and properties
   1. Fundamental constants
   2. Atomic and nuclidic masses
   3. Atomic radii
B. Atomic energy levels
   1. Energy levels, including Lande g-factors
   2. Ionization potentials and electron affinities
C. Atomic spectral data
   1. Emission spectral lines and intensities
   2. Absorption spectra-wavelengths and line shapes
   3. Absorption coefficients including photoionization
   4. Oscillator strengths (f values)
   5. Laser emission lines (atomic and molecular)
   6. Multiplet wavelengths, intensities, excitation potentials
   7. Hyperfine constants
   8. Names effects - Stark, etc.
D. Atomic and molecular X-ray spectral data
   1. Characteristic wavelengths and emission intensities
   2. Absorption spectra and critical potentials
E. Atomic and molecular collision data
   1. Heavy particle - heavy particle interactions; ionic reaction rates
   2. Electron - heavy particle interactions
   3. Field-induced phenomena
   4. Particle penetration through matter
F. Particle-surface interactions
G. Plasma properties
   1. Electronic and ionic transport phenomena

2. Line profile data-Stark broadening
3. Plasma resonance data
4. Recombination coefficients (review recommended)
5. Free-free absorption coefficients and capacities
6. Collision frequencies
7. Gaseous electronics
8. Plasma partition functions

H. Direct spectral data
1. Infrared spectra
2. Microwave spectra
3. Atlas of electronic spectra
4. Visible and UV absorption spectra including vacuum UV
5. Luminescence and related spectral data
6. NMR spectra
   a. High resolution
   b. Broad line
7. ESR spectra (organic and free radicals, gases)
8. Mass spectra
   a. Molecular masses
9. Raman spectra
10. Optical rotatory dispersion and circular dichroism

I. Information on molecular energy levels derived from spectral data-Diatomic molecules
1. A single table (similar to Herzberg) giving electronic levels and symmetries, vibrational constants, rotational constants, coupling constants, dissociation energies.
2. Diatomic potential curves for all known electronic states

J. Information on molecular energy levels derived from spectral data - Polyatomic molecules
1. Electronic energy levels
2. Vibrational fundamentals and vibrational levels
3. Force constants
4. Rotational constants
5. Chemical shifts and spin-spin coupling constants (to be combined with NMR spectra)
6. Miscellaneous magnetic coupling constants, g-factors, etc.
7. Ionization potentials, electron affinities, appearance potentials

K. Other well defined properties of atoms and molecules
1. Refractive index (spectral response)
2. Dielectric constants
3. Dipole moments (and higher moments)
4. Atomic and molecular polarizability
5. Magnetic susceptibility

(Critical review recommended to define the state of understanding and utility of additivity features of the above properties)

6. Interatomic distances and angles
7. Barriers to internal rotation
8. Non-linear optics
9. Kerr constants, Faraday effect data, etc.

L. Transition probabilities
1. Electronic f values
2. Photo-dissociation and radiative association, photo-ionization, photo-detachment rates; ionization efficiency curves
3. Virbrational overlap integrals (to be handled with I 1 and 2)

M. Descriptive chemical and analytical data
   1. Gas chromatographic values
   2. Pyrolysis patterns
   3. Differential thermal analysis data
N. Non-observable computed functions
O. Interatomic and intermolecular forces

IIIB Solid State
A. Optical Properties
   1. Spectroscopy of electronic systems
      Color centers
      Paramagnetic ions
      Absorption spectra of imperfection in semi-conductors
      I.R. spectra
   2. Electronic energy gaps
      Fundamental absorption edges
B. Electrical Properties
   1. Resistivity
   2. Superconductivity
C. Magnetic Properties
   1. Magnetic heat capacities
   2. Saturation moment
   3. Anisotropy
   4. Magnete striction
   5. Magnetic transitions
   6. Internal field (NMR spec.)
      a. Gyromagnetic ratio
      b. Hyperfine interaction
      c. Knight shift
      d. Chemical shift
D. Mechanical Properties
   1. Phonon spectra
      a. Lattice vibrations
   2. Acoustical properties
E. Thermal
   1. Densities
      a. Equation of state
      b. Measurement
      c. High pressure equation of state
   2. Higher order transitions
   3. Distribution coefficient
   4. Heat capacity
      a. Electronic
   5. Thermal conductivity

IV B Thermodynamic and Transport Properties

1. All standard thermodynamic quantities and functions
   H, U, S, A, Cp, Cv, Cs, $\frac{G^\circ - H^\circ_o}{T}$, $\frac{H - Ho^\circ}{T}$, $H_t - Ho^\circ$

2. Heats of:
   a. Adsorption
   b. Combustion
   c. Dilution
   d. Dissociation
   e. Formation
   f. Fusion
   g. Ionization
   h. Mixing
   i. Solution
      Integral
      Differential
   j. Sublimation
   k. Transition
   l. Vaporization
3. Electron affinity
4. Equilibrium constant
   Chemical equilibrium constant
   Decomposition
   Ionization constants
   Solubility product
   Stability constants for complex ions
5. Partial molar quantities
6. Apparent molar quantitities
7. Activities
   Activity coefficients
   Aqueous
   Non-aqueous
   Fused Salts
8. Solubilities
   Organic
   Inorganic
   Metals
9. Distribution coefficient
10. Emf Data
    Standard cell potentials
    Transference numbers
    Mobilities
    Junction potentials
    Hydration numbers
    Conductivities
11. PVT Data (General)
    Critical constants
    Critical data
    Density
    Equations of state
    Fugacities
    Joule-Thompson coefficients
    Inversion temperatures
    Lennard-Jones potentials
    Velocity of sound
    Virial coefficients
    Partition functions
    Compressibilities
12. Coefficients of expansion
13. Surface energies

14. Lattice energies
15. Croscopic constants
16. Phase relations
    - Solid - solid
    - Solid - vapor
    - Solid - liquid
    - Vapor - liquid
    - Liquid - Liquid
17. Membrane equilibria
18. Polarographic half-wave potentials
19. Osmotic coefficients
20. Viscosity
21. Density
22. Boiling points
23. Melting points

V B Colloid and Surface Properties

A. Colloidal systems

1. Lyophobic colloids
    a. Formation of sols: Precipitation kinetics, nucleaton and crystal growth
    b. Aging sols
    c. Particle size and shape
    d. Colloidal stability: flocculation values, flocculation kinetics, gelation, coalescence of emulsions
    e. Sedimentation and subsidence
    f. Osmotic pressures
    g. Swelling pressures
    h. Electrical double layer properties
    i. Electrokinetic properties (electrophoresis, sedimentation and centrifugation potentials
    j. Electrical properties (dielectric constant and conductivity of colloidal solutions
    k. Optical properties: light scattering, light absorption, electrooptical, and streaming birefringence
    l. Rheological properties
    m. Adsorption on colloidal particles
2. Lyophilic colloids
    a. Formation of sols: polymerication kinetics, solubility of macromolecular compounds
    b. Aging, breakdown of chains
    c. Molecular weight, coil dimensions
    d. Colloidal stability: coagulation, salting out, gelation, sensitization and protection of lyophobic colloids-gold numbers
    e. Sedimentation
    f. Osmotic pressure, diffusion
    g. Swelling pressures
    h. Electrical double layer properties, isoelectric point proteins
    i. Electrokinetic properties (electrophoresis, sedimentation and centrifugation potentials, electroviscous effect)
    j. Electrical properties (dielectric constant and conductivity of the sols and gels)

k. Optical properties (light scattering, light absorption, birefringence, refractive (index)
l. Rheological properties
m. Adsorption of polymers at interfaces
n. Solubility of gases in colloidal solutions

3. Association colloids
a. Critical micelle concentrations
b. Micellar weight
c. Solubility
d. Hydrolysis of soaps
e. Phase equilibria
f. Osmotic pressures-freezing point lowering, boiling point elevation
g. Electrical properties (dielectric constant and conductivity of the solutions)
h. Optical properties (light scattering, light absorption, refractive index)
i. Rheological properties
j. Surface tension of the solutions

B. Interfaces

1. Properties of interfaces
a. Surface total energies, enthalpies, entropies and free energies of solids and liquids. (Includes surface tension.)
b. Interfacial tensions
c. Contact angles
d. Diffusion and transport properties at surfaces, (heat transfer, mass transfer through interfaces and surface diffusion)
e. Electrical properties of interfaces: surface conductance, streaming potentials, electroendosmosis, liquid junction potentials, membrane potentials.

2. Adsorption at surfaces
a. Physical adsorption of gases and vapors on solids-adsorption isotherm. Molecular cross sectional areas of the adsorbates, specific surface areas of solids, pore structure of solids; Free energy, entropy and heat of physical adsorption; rates of adsorption
b. Adsorption of liquids on solids, adsorption from solution, adsorption isotherm. Molecular cross sectional area of adsorbed compounds; Free energy, entropy, and heat of adsorption.
c. Chemisorption. Free energy, entropy and heat of chemisorption; Physical properties of chemisorbed molecules.

3. Monomolecular films
a. Thickness of films and molecular cross sectional area. Equations of state of monomolecular films. Electrical potentials of surface films.

VI B Mechanical Properties
A. Crystalline substances
1. Single crystal
a. Linear behavior
(1) Elastic constants
(2) Temperature coefficients of
(3) Pressure coefficients of
(4) Anelastic relaxation strength (decrement)
(5) Temperature coefficients of
b. Non-linear behavior
(1) Critical resolved shear stress
(2) Temperature dependence of
(3) Slip crystallography
(4) Stress strain curves including strain-rate and temperature dependence
(5) Stacking fault energy (including impurity dependence)
(6) Dislocation velocity vs stress
(7) Thermal recovery
(8) Steady state creep-activation energy vs temperature
(9) Force-activation distance for logarithmic creep
(10) Creep curves vs temperature, stress parameters
c. Terminal behavior
(1) Fracture stress
(2) Surface energy
2. Polycrystalline metals and alloys
a. Linear behavior
(1) Modulus of elasticity in tension
(2) Modulus of elasticity in compression
(3) Modulus of elasticity in shear
(4) Proportional limit
(5) Poisson's ratio
(6) Bulk modulus
b. Non-linear behavior
(1) Stress-strain curves (engineering and true)
(2) Yield strength in tension
(3) Yield strength in compression
(4) Yield strength in shear
(5) Tensile strength
(6) Reduction in area
(7) Creep characteristics in tension
(8) Creep characteristics in compression
(9) Stress-relaxation in tension
(10) Hardness
c. Terminal behavior
(1) True stress at fracture
(2) True strain at fracture
(3) Elongation
(4) Reduction of area
(5) Stress rupture
(6) Fatigue strength

3. Polycrystalline Ceramics
   a. Linear behavior
      (1) Elastic moduli (bulk, shear, Young's modulus, Poisson's ratio) as a function of porosity. Zero porosity obtained by direct measurement or by extrapolation.
      (2) Temperature dependence of above elastic properties expressed as a fraction of the room temperature value (eliminates porosity) as far into the temperature range of grain boundary sliding as data permit.
      (3) Nabarro - Herring creep parameter as a function of temperature. Activation energy when available.
      (4) Internal friction parameters and relation to structural defects.
   b. Non-linear behavior
      (1) Stress-time curves at constant strain rate and temperatures, for various strain rates and temperatures.
      (2) Creep curves under constant load.
   c. Terminal behavior
      (1) Fracture stress as a function of porosity and grain size. Surface condition effects when data available. Temperature and stress rate dependence. Effect of atmosphere.
4. Crystalline Polymers
   a. Linear behavior
      (1) Curves for the real and imaginary parts of the bulk and shear modulus at various frequencies and over a wide temperature range. These should be presented in review articles which stress the physical and chemical characterization of the samples on which measurements have been made.
   b. Non-linear behavior
      (These are not understood well enough on either the basic theoretical level or the experimental level to merit their inclusion.)
   c. Terminal behavior
      (1) A critical review article on the relationship of the terminal properties of fibers to fundamental aspects of the structure.

B. Non-Crystalline Substances
1. Inorganic glasses
   a. Linear behavior
      (1) Elastic moduli at thermal equilibrium (bulk moduli at infinite and at zero frequency, shear modulus at infinite frequency). Relaxation times, their distributions and associated change in moduli.
      (2) Elastic moduli (bulk, shear and Young's moduli. Poisson's ratio) at room temperature for glasses of specified fictive temperature.
      (3) Viscosity (shear) as a function of temperature at thermal equilibrium. Softening, strain, glass transition and annealing temperatures.
      (4) Viscosity as a function of temperature and thermal history.
      (5) Ratio of volume to shear viscosity.
      (6) Internal friction parameters (fiber torsion and other techniques).
   b. Non-linear behavior
      (1) Pressure dependence of bulk modulus.
      (2) Viscosity (if enough data on non-linear behavior exists.
      (3) Knoophardness

c. Terminal behavior
   (1) Surface tension as a function of temperature
   (2) Fracture energy and attempts to relate to surface energy
   (3) Modulus of rupture
   (4) Crack propagation velocity

2. Organic glasses
   a. Linear behavior
      (1) Glass transition temperature
      (2) Thermal expansion coefficient (below, but near T_g)
      (3) Compressibility (below, but near T_g)
   b. Non-linear behavior
      Nothing at present
   c. Terminal behavior

3. Polymer liquids
   a. Linear behavior
      (1) Viscosity as a function of temperature, pressure and molecular weight. (Review and tables.)
      (2) Limiting (high frequency) modulus as a function of temperature and pressure.
      (3) Glass transition (Same as B.2)
      (4) Intrinsic viscosity functions for each polymer in one or more solvents is important information as is also information on chain length, end-to-end distance, etc. (Such information should be covered somewhere by NSRDS. This might be a good place).
   b. Non-linear behavior
      Nothing now.
   c. Terminal behavior
      (1) Critical review with representative curves and/or tabulations

4. Simple liquids
   a. Linear behavior
      (1) Viscosity as function of temperature and pressure
      (2) Surface tension
      (3) Limiting (high frequency) values of shear rigidities as function of temperature and pressure.
   b. Non-linear behavior
      Nothing at present
   c. Terminal behavior
      Nothing at present

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