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your organization of our activities.

Thanks are extended to all those who responded to our Questionnaire of 26 December 1968. The answers received will be very helpful.

Guy Waddington

GW/s
enclosures

cc: Dr. Martin Paul
Mr. Nathan E. Promisel
Dr. G. C. Sponsler
Dr. C. E. Sunderlin
Mr. George Wood
Dr. Hugh Odishaw
Dr. Joseph W. Berg, Jr.

PROCEEDINGS

of the

OFFICE OF CRITICAL TABLES ADVISORY BOARD MEETING

held at the

National Academy of Sciences

18 November 1968

with reports on the

NATIONAL BUREAU OF STANDARDS

NATIONAL STANDARD REFERENCE DATA PROGRAM

National Academy of Sciences - National Academy of Engineering
National Research Council
2101 Constitution Avenue, N. W.
Washington, D. C. 20418

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FOREWORD

This report presents the complete Proceedings of the Meeting of the Advisory Board of the Office of Critical Tables of the National Research Council held at the National Academy of Sciences in Washington, D. C. on November 18, 1968.

Morning and afternoon sessions provided a full day for the Board. The morning session was designed for review of recent work of the Office of Critical Tables, with international developments being singled out for special attention. Contributions to data compilation work from the private sector of American science and technology with emphasis on contributions from industry were also featured. The afternoon session was devoted to the presentation, by the Director and Staff of the Office of Standard Reference Data of the National Bureau of Standards, of the story of the growth of the National Standard Reference Data Program since 1963. It is clear that, from the small beginning in 1957 of the Office of Critical Tables, there has developed a strong momentum that will bring more and more reliable numerical data for scientists and engineers in the United States, and that the basis has been established for worldwide participation in this important work through the Committee on Data for Science and Technology of the International Council of Scientific Unions.

Frederick D. Rossini
Chairman of the Executive Committee
Office of Critical Tables
National Research Council

PROGRAM

Morning Session

Remarks by the Chairman, Allen V. Astin, Director, National Bureau of Standards

Welcome by C.E. Sunderlin, Special Assistant to the President, National Academy of Sciences

The Role of the National Research Council in Critical Tables of Standard Reference Data by Frederick D. Rossini, Chairman, Executive Committee of the Office of Critical Tables

Report to the Advisory Board by Guy Waddington, Director, Office of Critical Tables

The ICSU-UNESCO Central Committee for a Study of World Science Information Systems, by Burton W. Adkinson, Head, Office of Science Information Service, National Science Foundation

Worldwide Organization for the Preparation and Dissemination of Critical Tables for Science and Technology by Frederick D. Rossini, President, Committee on Data for Science and Technology of the International Council of Scientific Unions

Numerical Data for Engineering and Technology:

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(b) The Process Industries: H. Heinemann, Advisory Board Representative for the Industrial Research Institute

(c) Analytical Data for the Metals Industry: W.L. Fink, Advisory Board Representative for the American Society for Testing and Materials

(d) Mechanical Properties Data for the Metals Industry: Taylor Lyman, Advisory Board Representative for the American Society for Metals, and Frank Speight for the Metal Properties Council

(c) Discussion on Data for Engineering and Technology

PROCEEDINGS OF THE MEETING

Morning Session

Chairman, Dr. Allen V. Astin

DR. BRODE: I now call to order this meeting of the Advisory Board of the Office of Critical Tables.

I am Dr. Robert Brode, (not my twin brother Wallace) and will serve as chairman pro-tem until Dr. Astin arrives. He will give his opening remarks at an appropriate time later in the program.

Dr. Gene Sunderlin, Special Assistant to Dr. Seitz, President of the National Academy of Sciences, will bring you greetings on behalf of the Academy.

WELCOMING REMARKS

By

Dr. C. E. Sunderlin

Special Assistant to President Frederick Seitz

DR. SUNDERLIN: Thank you, Dr. Brode.

Members of the Advisory Board, it is a great pleasure to welcome you on behalf of President Seitz and the Academy.

As Bob has said, I am substituting for President Seitz but this in no way diminishes the warmth of the welcome that we extend to you today.

Guy Waddington told me, in answer to a question, that these meetings of the Advisory Board will take place every three years. However, the last meeting took place five years ago and I think that the reason for his answer is that the three-year interval represents a new policy to accord with the three-year term of office of Members.

Three years from now it is hoped that this meeting of the Advisory Board will occur in the new Dryden Auditorium which we expect will be completed and ready for use in about two years. The new auditorium will seat about 750 people, will provide office space, and will greatly increase the utility of the Academy buildings for meetings of all kinds.

I would like to mention two things in connection with your work which seems to me to be of particular significance. The first is the National Standard Reference Data Program of the National Bureau of Standards which about five years ago, if I remember correctly, was just beginning. Thanks to the good work of Ed Brady, Fred Rossini, and many others in the audience, the Standard Reference Data Program has gotten off the ground. I am also glad to say -- if my information is correct -- that the program has been legitimatized. By that I mean that Congress has finally passed legislation that gives recognition to the program so that hopefully the representatives of the Bureau of Standards and the Department of Commerce will not face the difficulties before appropriations committees that they have experienced in the past.

The second comment refers to what is now called CODATA, the Committee on Data for Science and Technology of the International Council of Scientific Unions, which also has gotten its program off the ground although there may still be problems in the early stages of its flight.

I think that the Office of Critical Tables and members of its Advisory Board should be congratulated on your part in these two significant developments during the last five years. I wish you a successful and profitable meeting.

DR. BRODE: We will hear next from Fred Rossini, Chairman of the Executive Committee of the Office of Critical Tables.

THE ROLE OF THE NATIONAL RESEARCH COUNCIL IN CRITICAL TABLES OF STANDARD REFERENCE DATA

By

Dr. Frederick D. Rossini, Chairman
Executive Committee of the Office of Critical Tables

Mr. Chairman, Members of the Advisory Board of the Office of Critical Tables of the National Research Council, and Guests.

In reporting on "The Role of the National Research Council in Critical Tables of Standard Reference Data", I want first to present a picture of the role of the National Research Council in the scientific-technical community of the country as a whole.

The National Research Council was established in 1916 as an instrumentality of the National Academy of Sciences, for the purpose of encouraging a broader participation of the scientists and engineers of the United States in the Academy's service to our country and of bringing into cooperation the scientists and engineers of industry, universities and government.

In 1918, President Woodrow Wilson requested the National Academy of Sciences to perpetuate the National Research Council, and outlined its purposes. These purposes were brought up to date in an executive order issued by President Eisenhower in 1956, which listed six objectives. It is important for us to note the sixth objective so listed, which reads:

"To gather and collate scientific and technical information, at home and abroad, in cooperation with governmental and other agencies, and to render such information available to duly accredited persons."

With the recent establishment of the National Academy of Engineering, the National Research Council is now an instrumentality of both the National Academy of Sciences and the National Academy of Engineering. The National Research Council mobilizes the knowledge, experience, and wisdom of the scientific-technical community of the United States, including the industrial, university and government sectors, for the solution of important problems. The Members of Committees of the National Research Council are chosen from the scientific-technical community because of their particular expertise in given areas and serve without pay but are reimbursed for expenses.

The Members of the Staff of the National Research Council and its Offices and Committees serve as the mechanism whereby the knowledge, experience and wisdom of the scientific-technical community are brought to bear on any given problem. Any report or publication emanating from a given Committee of the National Research Council must represent the consensus of the opinions of all the Members of the given Committee and must be developed by the process of accumulating facts, developing policy statements, and achieving concurrence through the circulation of preliminary drafts and the final version of the given report or publication. The National Research Council provides the Staff work required to carry on all of these activities.

In its reports on the various problems and works that come before it, the National Research Council serves as the spokesman for the scientific-technical community of the country. The National Research

Council serves and coordinates the interests of the industrial, university, and government sectors of our scientific-technical community. Through the Foreign Office of the Academy, the National Research Council maintains links with appropriate international organizations, including the International Council of Scientific Unions and its Member Unions.

With this background, I would like now to develop the story of the role of the National Research Council in the matter of critical tables of standard reference data for science and technology.

In 1919, three years after the establishment of the National Research Council, the International Union of Pure and Applied Chemistry at a meeting in London, England, gave birth to a new project, the International Critical Tables of Numerical Data of Physics, Chemistry, and Technology. For this project, the United States was assigned the financial and editorial responsibility. The National Academy of Sciences-National Research Council accepted the executive, editorial, and financial responsibilities for the United States. With the cooperation of industry, the American Chemical Society, and the American Physical Society, the Academy created a Board of Trustees to take charge of the financial and business administration and established a Board of Editors to supervise the preparation of the tables proper. Edward W. Washburn, one of the leading physical chemists of our country at that time, became Editor-in-Chief. The entire enterprise was made possible by a fund of $200, 000 contributed largely by approximately 200 industrial companies of the United States. Meanwhile, in 1923, at a meeting in Brussels, Belgium, the then International Research Council, now the International Council of Scientific Unions, gave its patronage to the project.

This famous collection of numerical data, the International Critical Tables under the leadership of Washburn, was the result of cooperative efforts by more than 400 scientists in 18 different countries. Seven volumes, with a total of approximately 3500 pages, were published in the years 1926 to 1930, with a separate index volume following in 1933. It was hoped that the International Critical Tables would become a continuing operation, with revisions and supplements from time to time, but, unfortunately, Washburn died in 1934 and this continuity never came to pass. The importance of the International Critical Tables to the science and technology of the world is evident from the fact that a significant number of sets of these tables are still being sold today - 42 years after their original issue.

About 1940, the National Research Council established a Committee on Tables of Constants. Although this Committee did consider it desirable to have a revision of the International Critical Tables, it saw no ready solution to that problem. This Committee devoted its efforts to the supervision of two data-compiling projects - one on chemical kinetics data and one on nuclear data.

About 1954, this Committee, under the new Chairmanship of Allen V. Astin, then also Director of the National Bureau of Standards, appointed an Ad Hoc Subcommittee charged with the task of recommending a definite course of action regarding the large and important overall job of providing numerical data for science and technology in the United States.

This Ad Hoc Subcommittee presented a report which was accepted by the parent Committee and included the following statements and recommendations:

1. There was no hope of repeating the work of the International Critical Tables as one large compilation job, for the following reasons:

a. Science and engineering have areas that never existed before, requiring totally new data;

b. The previously known areas of science and engineering have expanded greatly in size, requiring many times more data than before;

c. The precision of measurement in science, and the precision of manufacturing in industry, have been pushed to a new magnitude, requiring more accurate data of greater precision.

d. An adequate and complete revision and extension of the International Critical Tables would today cost perhaps 200 times as much as the original job - namely, upwards of $40,000,000, and, further, provision for continuity would be required, - an important element lacking in the organization of the International Critical Tables.

2. From 1938 to 1955, other data-compiling projects, operating on a continuing basis, had come into existence in the United States. These projects together involved total expenditures of more than one million dollars per year, and included the following, among others:

a. The American Petroleum Institute Research Project 44 on physical, thermodynamic, and spectral properties of hydrocarbons and related compounds.

b. The Manufacturing Chemists Association Research Project on physical, thermodynamic, and spectral properties of chemical compounds;

c. The U. S. Atomic Energy Commission Project on nuclear data;

d. The U. S. Bureau of Mines Project on thermodynamic data on metallurgical compounds;

e. The Purdue University Center on Thermophysical Properties;

f. The Dow Chemical Company Project on thermodynamic properties of selected compounds;

g. Several National Bureau of Standards Projects on thermodynamic, on atomic, and on other properties of a large variety of compounds.

Any new overall plan for replacing the International Critical Tables would have to take the foregoing operating projects into consideration.

The report concluded that a new plan should be provided and recommended the establishment under the National Research Council of an Office of Critical Tables, with appropriate responsibilities. The report was accepted by the National Academy of Sciences-National Research Council.

In 1957, the National Research Council established the Office of Critical Tables, with the following objectives:

1. To survey the needs of science and industry for critical tables of numerical data.

2. To stimulate and encourage existing continuing data-compiling projects.

3. To promote uniform editorial policy and procedures, with the use of internationally approved constants, units, and symbols.

4. To provide a directory-survey of continuing data-compiling project.

5. To assist in establishing needed data-compiling projects for new scientific areas, with financial support.

Within the National Research Council, the Office of Critical Tables was set up as a joint responsibility of four Divisions: Engineering, Earth Sciences, Physical Sciences, and Chemistry and Chemical Technology, with the latter handling the administrative work.

In line with the objectives listed above, the Office of Critical Tables functions in an advisory capacity to stimulate and encourage work on continuing data-compiling projects in all sectors of the scientific and technical community of the United States, including both government and non-government areas.

Also, the Office of Critical Tables serves as the link between the United States and other countries and Unions through the International Council of Scientific Unions. In particular, it provides the input to the International Council of Scientific Unions' Committee on Data for Science and Technology, or CODATA as it is called, including material for the important world-wide compendium-directory-survey of continuing data-compiling projects and related material.

The Office of Critical Tables has at present an Executive Committee of seven Members, including the Chairman, the Director of the National Bureau of Standards ex-officio, one representative each from the National Research Council Divisions of Physical Sciences, Earth Sciences, and Chemistry and Chemical Technology, and two representatives from the National Research Council Division of Engineering. We hope to add an additional Member from the Division of Engineering.

Also, the Office of Critical Tables has a large Advisory Board comprising one representative from each of the major societies and associations, together with a number of experts in the field.

We are fortunate that our Office of Critical Tables is a part of the National Research Council, operating under the National Academy of Sciences and the National Academy of Engineering, since we benefit from the prestigious qualities of these organizations.

The National Research Council has permanence, is impartial in operation, has contacts with all scientific and technical organizations of the United States, and has channels of communication with scientific and technical organizations of other countries and with the

International Council of Scientific Unions and its Member Unions.

The National Research Council, operating under the National Academy of Sciences and the National Academy of Engineering, has the prestige needed for the successful implementation of a task involving cooperation of various segments, both private and government, of the scientific and technical community of our country.

In the fall of 1957, exactly eleven years ago, Guy Waddington left his position as Director of the Thermodynamics Laboratory of the Bureau of Mines at Bartlesville, Oklahoma, to come to the National Research Council here to start up the new Office of Critical Tables. In his report to you this morning, Guy Waddington will summarize all that has happened in his ten years of operation of the Office of Critical Tables.

DR. ASTIN: Thank you very much, Dr. Rossini, for a most illuminating report on the interest of the National Research Council in critical data compilation.

We are next privileged to hear a report from the NRC's Office of Critical Tables, Dr. Guy Waddington.

REPORT TO THE ADVISORY BOARD

By

Dr. Guy Waddington, Director
Office of Critical Tables

Professor Rossini, Chairman of the Executive Committee of the Office of Critical Tables, has reviewed for you the history, philosophy and actions which led to the formation of the Office of Critical Tables in 1957. My purpose in reporting to the Advisory Board is to review in outline form the story of the progress made since the start-up of the Office, to indicate the mechanisms that now exist to carry the work forward, to tell something of the present functions of OCT, and to indicate the direction of future effort.

Background: To present a coherent story it is necessary to refer to the state of affairs in 1955 and to the original aims of the Office of Critical Tables which Professor Rossini has indicated. First, the underlying plan has to be grasped. The conditions existing in 1955 on which the overall plan was based were about as follows: (a) The magnitude of the task of critically evaluating and publishing all existing properties had become far too large to do in one center. Decentralization of effort was necessary; (b) A number of excellent small centers existed; (c) Many more centers were needed; (d) Quality and continuity had to be built into any new centers created; and (e) Informal coordination among these would be desirable.

To illustrate the kinds of centers which already existed in 1955 the following can be mentioned: (a) NBS Circular 500 (thermodynamic data); (b) American Petroleum Institute RP44 (thermodynamic and spectral data); (c) Dana's System of Mineralogy; (d) NRC Nuclear Data Project; (e) ASTM Powder Diffraction Data; (f) NBS Atomic Energy Levels; and (g) Landolt-Börnstein Tabellen.

Among the foregoing, (a) and (f) were in a governmental organization; (b) and (e) were operated by industrially oriented groups; (c) is conducted at Harvard University and has existed since 1837; (d) has since been transferred to the Oak Ridge National Laboratory; and (g) which in the past has covered all areas of physical science in a number of multi-volume editions will become a monograph series after the Sixth Edition is complete.

A few remarks to establish the kinds of data included in the work of OCT are in order. Numerical data can be divided into approximate categories, such as the following: (a) Well defined properties of characterized pure substances; (b) Properties of characterized simple systems; (c) Properties of engineering materials; (d) Arbitrary parameters for industrial and natural products; and (e) Data for large natural systems.

By defined properties under (a) we mean conventional well behaved properties such as density, entropy, infrared spectra, etc., which are inherent characteristics of pure substances. Well characterized systems of substances as in (b) also possess properties which can be rigorously specified and accurately determined. Most of the data of physics, chemistry and their subdivisions are included under (a) and (b). In (c) we are referring to the same type of properties, but the systems are complex and not easy to characterize and to reproduce. In (d) a new note is introduced in that the property concept is less clear.

For example, the hardness of a substance is usually presented on an arbitrary scale and its value is a function of a particular carefully defined method of measurement. Many test methods used in industry are of this type. The areas under (e) include data for meteorology, oceanography, much of astronomy and so on. In the biological sciences many types of numerical data are encountered and these may be of one or the other of the foregoing types.

In the beginning it was clear that types (a) and (b) of data would comprise the prime target of OCT; but it was recognized as did the International Critical Tables (Vol. 2) that industry has extremely important needs, and also that for the long term the data of large natural systems should be kept in mind.

OCT Objectives: With the foregoing background of ideas and facts the Executive Committee of OCT decided that the work of the Office should be directed to the following objectives which Professor Rossini has stated but which I will repeat in a somewhat different way: (a) Identify all centers that meet quality standards and publish a directory of such centers; (b) Informally coordinate and encourage existing projects; (c) Encourage formation of new projects; (d) Promote high standards and compatability of products; and (e) Provide a central indexing service.

Now let us examine what has happened in implementing these five aims. Items (a) and (b) are parts of the same objective - namely, the identification of what is going on. The summation of these efforts is available in the three separate books: (1) Directory of Continuing Numerical Data Projects, Publication 837, National Academy of Sciences, National Research Council, Washington, D. C., 1961. (2) Continuing Numerical Data Projects, a Survey and Analysis, Publication 1463, National Academy of Sciences-National Research Council, Washington, D. C., 1966. (3) International Compendium of Numerical Data Projects to be published in early 1969 under the auspices of the ICSU Committee on Data for Science and Technology. The total entries in these three volumes were 43, 73 and 153 in the years 1961, 1966 and 1969 respectively. Recent growth is impressive. Each center represents one or a number of scientists evaluating and compiling data in a given field.

The relative emphasis on various fields of science is indicated by the fact that of the 73 entries in the 1966 volume 19 entries were on thermodynamic and related fields, 11 on crystallography, 9 on nuclear science and 29 on various areas of spectroscopy.

It is knowledge of what centers exist, what they are doing and how they do it, where they are and how supported, and so on that makes possible a rational attack on the job that needs to be done. Thus the directories are extremely important to the whole effort.

Now turning to the mission of OCT to stimulate and encourage existing centers, this objective can be approached in various ways. For example, in the early years of OCT, I, as a representative of the OCT, visited many centers in the U.S. and abroad and perhaps contributed to a feeling on the part of directors of projects and their staffs that they were helping science in an important way and were part of a community doing similar work in different parts of the world. Also papers have been written and talks given by Prof. Rossini and me in many places such as Vienna, Lund (Sweden), Madrid, Tokyo, Osaka, Kyoto, Leningrad, Moscow and London in addition to many audiences in the U.S. More recently staff members of the Office of Standard Reference Data, with talks given in many places, have been extending awareness of the numerical data problem to a large number of people. But perhaps the most effective method of stimulation is the organization of conferences to be attended by all or most of the world's experts and also by newcomers to compiling work. OCT did not organize all the following conferences, but did start a trend which now continues almost spontaneously with some help and participation on our part:

1. Gordon Research Conference on Information Processing for Critical Tables of Scientific Data, New Hampton, N.H. (1960).

2. Gordon Research Conference on Scientific Information Problems in Research: Critical Tables and Progress in Science, New Hampton, N.H. (1964).

3. Gordon Research Conference on the Numerical Data of Science and Technology - Its Generation and Critical Evaluation, Enumclaw, Washington (1966).

4. Symposium on Compilations of Data on Chemical and Physical Properties of Substances, 152nd National Meeting of the American Chemical Society, New York, N.Y. (1966).

5. Discussion Meeting on Data for Science and Technology, The Royal Society, London, England (1967).

6. First International CODATA Conference, Arnoldshain, Germany, (1968).

7. Gordon Conference on Numerical Data for Science and Technology, Tilton, N.H. (1969).

8. International Symposium on Data for Science and Technology, Warsaw, Poland, sponsored by the Polish Academy of Sciences (1969).

9. Second International CODATA Conference, U.K. (1970).

The result of these various efforts to stimulate and to improve communications is that there are now many experts in the world working toward similar goals. The many, many discussions and meetings have resulted in improved methodology, avoidance of overlap, and division of labor. Quality of effort too has been improved which brings us to another of the OCT objectives, namely, the stimulation of high standards.

We have hammered incessantly on the idea that compilers must use internationally recognized symbols, nomenclature, fundamental constants and so on. And, that all quantities tabulated must be rigorously defined, that uncertainties in numerical values should be suitably indicated, that general methods of evaluation should be presented in sufficient detail and that all literature sources of information involved in the evaluation and selection progress should be revealed by specific references. But frequently the guidelines needed by compilers have been missing, imperfect or out-of-date.

Two special examples of such deficiencies came to light in 1960 when it was observed (1) that compilers were using a variety of sets of fundamental constants, each one consistent within itself, but differing from the others in significant ways thus leading to nuisance levels of incompatibility between compilations; and (2) that the U. S. A. was not participating effectively in the work of Technical Committee 12 of the International Organization for Standardization. TC/12, since 1952, with participation by all major countries, has been developing recommendations of consistent and coherent symbols, terminology and units for all major areas of science.

To improve the fundamental constants situation an interdivisional NRC Committee on Fundamental Constants was established under the auspices of the Executive Committee of the Office of Critical Tables. This new Committee, composed of leading experts, in 1963 recommended a new set of constants, incorporating the results of the then new redeterminations of several constants. The formulation of the set of constants was largely the work of J. W. Du Mond and E. R. Cohen. It was subsequently given tacit approval by the International Union of Pure and Applied Physics, and the International Union of Pure and Applied Chemistry. It can be interpolated here that improvements in accuracy of measurements of several basic constants have occurred since 1963 and first steps toward a new formulation are now being taken.

Regarding U. S. participation in efforts to obtain international agreement on symbols for all areas of the physical sciences, the following was done. First, an interdisciplinary NRC Committee on Symbols, Units and Terminology was established under the aegis of the Executive Committee of the Office of Critical Tables. Then, on request from the American Standards Association (now the U. S. A. Standards Institute), the new committee became the U. S. Committee Advisory to Technical Committee 12 (TC/12) of the International Organization for Standardization (ISO). This Committee has functioned effectively in reviewing TC/12 draft documents; and its chairman, Dr. Hugh Wolfe of the American Institute of Physics, is a Member of the TC/12 planning committee. This accomplishment has been a key factor in bringing about excellent communications among several U. S. committees responsible for units and symbols and between these committees and their international counterparts in ISO, IUPAC, and IUPAP.

Another kind of guideline of great importance to compilers is addressed to the author of primary research papers. Scientists in three disciplines have now prepared carefully thought-out instructions to the authors of primary research papers. The purpose of these instructions is to make sure that the author includes in his paper all facts necessary for an evaluation of his work and of the numerical results he has presented. The three publications are:

> Resolution on the Publication of Calorimetric and Thermodynamic Data, Physics Today, February, 1961.
>
> Specifications for Evaluation of Infrared Reference Spectra by the Coblentz Society Board of Managers, Anal. Chem., Vol. 38, No. 9, August 1966, 27A.
>
> Primary Crystallographic Data, O. Kennard, J. C. Speakman and J. D. H. Donnay, Acta Cryst. 22, 445 (1967).

OCT has consistently encouraged groups of experts, through society committees, or commissions of international unions, to prepare and disseminate widely such guidelines. We feel strongly that other groups of specialists could and should perform similar services for workers in their fields.

Other encouraging signs of greater awareness, on the part of U. S. organizations, of the importance of standardizing fundamental aspects of scientific communication may be mentioned. The National Bureau of Standards has endorsed the International System (SI) of units and promotes its use in its own publications as does also the Institute of Electrical and Electronic Engineers. The American Society for Testing and Materials, and Engineering Joint Council are also moving in the same direction. The American Chemical Society has recently published a Handbook for Authors of papers in all of its journals. This handbook reflects a move toward the use of internationally accepted units but leaves considerable discretion to the editors and authors. It is a big step forward in which OCT is pleased to have had a small part.

Turning now to another OCT task you will recall that OCT considered establishing a central index to the content of all publications meeting quality standards. This idea was placed in abeyance after a combined index for 6 key thermodynamic publications was produced. Such a program is beyond the capabilities of a small group. The concept of a central index on tape keeps coming up but no one at this time has the resources to do the job. The best that I can suggest to help this situation is that compilers pay attention to good indexing of their products and possibly to methods of indexing compatible with those of other centers.

There is one important original aim of OCT which I have not discussed, namely, the encouragement and establishment of new projects. It turned out that this task was beyond the resources of OCT and was a management and funding job of considerable magnitude. This realization was a factor behind the establishment of the Office of Standard Reference Data in NBS in 1963 as a result of a directive from the Office of Science and Technology. Dr. Brady will report to you this afternoon on the development of the National Standard Reference Data Program since its formation in 1963 and I believe you will find it an interesting and impressive story.

I would now like to remind you of the time scale on which progress has been made with the evaluation and publication of critical tables of standard reference data. We may select the following dates as turning points in the evolution of mechanisms for moving forward with the large task of evaluating and publishing data for all of science:
(a) The International Critical Tables was initated (by IUPAC) in 1919;

(b) The International Critical Tables were completed (by NAS) in 1933; (c) The National Research Council Committee on Critical Tables was established in 1955; (d) The National Research Council Office of Critical Tables was established in 1957; (e) The National Bureau of Standards Office of Standard Reference Data was established in 1963, and (f) The ICSU Committee on Data for Science and Technology (CODATA) was established in 1966.

Professor Rossini will report in detail on the ICSU-CODATA activity started in 1966 which is a focal point for widespread international participation in compiling numerical data. But from the listing (a to f), it is clear that there is now a framework of organizations to begin coordinating the fiscal and intellectual resources of governments and of the scientific communities in all major countries and international unions.

Advisory services: The OSRD and CODATA developments have brought new functions to OCT. OSRD has of course taken over the task of organizing and funding new compilation projects in government, and to a considerable extent in the private sector. The problem of establishing priorities, the need to find experts for compiling projects, and the need to establish policies consistent with the requirements of scientists and engineers have caused NBS to ask OCT for advisory services of several kinds. These services are not as yet fully implemented but the pattern is as follows: (a) The Executive Committee of OCT serves as the overall Advisory Committee for the OSRD. It meets about once a year to review broadly the progress of the program and submits a report to OSRD containing recommendations on policy matters. (b) Next, advisory panels will be provided for each of the seven sections of the NSRDP. The panel on Atomic and Molecular Properties is fully operational under the chairmanship of E. U. Condon. Panels for other areas have met informally, but are not yet officially established. (c) Thirdly, ad hoc panels will be used rather liberally by OCT on request from OSRD to examine specific areas of science that seem to require attention. Such ad hoc groups in recent months have considered NMR and laser-excited Raman spectra, and the digitizing of spectra. Reports with recommendations are submitted to OSRD after each meeting.

International activities: Since 1964 OCT has devoted much time to the Committee on Data for Science and Technology - in two steps. From 1964 to the formation of CODATA in January 1966, OCT, with its Executive Committee, provided backup to the U. S. part of the effort to get CODATA started. In this connection, sincere thanks are due to Harrison Brown, Foreign Secretary of the Academy, and his able lieutenant E. C. Rowan, and other members of the staff of the Office of the Foreign Secretary, for the parts they have played in this effort. After CODATA was established in 1966 to the present, OCT has served CODATA in various ways. In addition to attempting to transfer some of its experience and knowledge to the new program, it provided quarters in the NAS for the Central Office for two years prior to its move to Frankfurt. Special aspects of the collaboration of OCT with CODATA include the following:

(a) Its Executive Committee has acted as the United States National Committee for CODATA and has provided valuable backup for the U. S. National Representative for CODATA.

(b) Its resources of knowledge, its files of information on projects, both in the U. S. and abroad, have provided a great deal of the input for the CODATA worldwide survey of data projects. OCT has produced and is now putting finishing touches on copy for the approximately 300 page book "International Compendium of Numerical Data Projects" to be published by a German publisher in early 1969.

(c) Specialized knowledge about scientists and projects helpful to the data cause is still feeding, through the U. S. National Member, into the operations of CODATA.

(d) And finally, channeling from CODATA through the U. S. National Member, awareness of CODATA activities is available to the OSRD and is very valuable to it in coordinating its activities with those in other countries.

Summary: I have given you only highlights of our activities. It is impossible to compress the multitude of small activities, many on the level of personal diplomacy, into a 25-minute report. I would now like to summarize for you the main directions of OCT as we see them. The broad mission is to do everything possible, in ways appropriate to the NAS, to help science and technology to satisfy their needs for reliable numerical data. Obvious directions of work include:

(a) To help provide strong and meaningful U. S. participation in the effort to obtain worldwide cooperation in compressing the numerical data of science into tables of critically evaluated standard reference data.

(b) To provide advisory services to the OSRD in its important task of operating the National Standard Reference Data System, bringing to this service the resources of the NAS-NAE-NRC.

(c) To continue to encourage and help the private sector of the country in carrying out portions of the task which are neither in governmental organizations nor funded from governmental sources. Many needs of the engineering sector are in this domain.

(d) And finally, to continue to use its influence to assure compilations of the highest quality and usefulness.

To summarize and close I will remind you that OCT is a relatively small organization. Its staff over the years has averaged three professionals, two of them at the PhD level, and two supporting staff members. The office depends heavily on the unselfish help and dedication of its Executive Committee. And lastly, I wish to recognize and thank the Office of Science Information Service of the National Science Foundation for early financial support and continuing encouragement, and also the NBS Office of Standard Reference Data for its more recent funding of the activities of the Office.

DR. ASTIN: Thank you very much, Dr. Waddington, for an interesting report on the interests, activities, and achievements of the Office of Critical Tables.

Our next background report concerns a study of world science information systems that is being undertaken by a committee set up by the International Council of Scientific Unions and UNESCO. To tell us about that, we have the Head of the Office of Science Information Service of the National Science Foundation, Dr. Burton W. Adkinson.

THE ICSU-UNESCO CENTRAL COMMITTEE FOR A STUDY OF WORLD SCIENCE INFORMATION SYSTEMS

By

Dr. Burton W. Adkinson, Head
Office of Science Information Service
National Science Foundation

DR. ADKINSON: Mr. Chairman, Ladies and Gentlemen:

My topic today is somewhat peripheral to the subject of critical data, but the organizers of this meeting thought it would be useful to hear about it because it deals broadly with scientific information at the international level in a manner paralleling the CODATA effort.

I would like first to start with a brief review of how the ICSU-UNESCO Central Committee came into being. At a Pugwash Conference in 1964 a resolution was passed urging the establishment of a world center to collect all scientific and technical information and make it generally available to all scientists in all countries. A few people in various countries were concerned about that resolution, because no one center could respond to world-wide demands for services.

Shortly after the Pugwash meeting UNESCO and ICSU began informal discussions to determine how UNESCO could obtain from ICSU advice on their various science programs. These discussions led to the formation of an ICSU-UNESCO Committee through which a small working group could survey the problem of a world information system and the need for a world center. A working group, consisting of six people, was convened in January 1967. They were asked to define the scope of, and to suggest topics for, a study. They were also asked to identify additional candidates for membership in an enlarged group. Dr. Harrison Brown, Foreign Secretary of the U.S. National Academy of Sciences, was the convenor of both groups. In addition to the original six people (Professor Boutry--France; Dr. Dainton--U.K.; Dr. Kaiser--Germany; Dr. Kotani--Japan; Professor Arutyunov--USSR, and myself), representatives from several other organizations were asked to participate as observer-advisers. These included representatives of international organizations and of various operating services throughout the United States and the world.

The group developed a statement limited to give major points, namely: (1) to examine only those information problems related to basic natural sciences as represented by the ICSU unions; (2) to consider ways and means of improving voluntary and flexible cooperation among existing and future information services; (3) to suggest ways and mean s of sharing tasks and information among the services in the different disciplines in the different countries; (4) to identify areas in which there could be developed standards and guidelines to facilitate transferability and selectivity; and (5) to pay special attention to the availability of scientific and technical information for developing countries. This fifth item, of course, is close to the heart of UNESCO which has many members from the developing countries.

As a result of this Working Group meeting a decision was made to support a study committee. No timetable was given to the committee, although there was an informal understanding that it might complete its assignment by 1970-1971. To show the interest of UNESCO and ICSU in this study, UNESCO reprogrammed its funds (with considerable difficulty in the middle of a fiscal period) and provided $35, 000 or $50, 000 and assigned a staff person to the committee. ICSU itself reprogrammed its funds and contributed about $10, 000 (a very substantial contribution for an international organization such as ICSU). ICSU regards this activity as a most important effort, and they are giving it their enthusiastic support.

Difficulty was experienced in deciding on a suitable name for the Committee. Initially it was called the "Central Committee for the Study of the Feasibility of Worldwide Information Systems." That was too complicated, so they decided on "World Information Systems in Science and Technology (WISSE)," but this also did not last. Now it has been given the arbitrary name of UNISIST and that is what we will call it.

Now let me tell you more about the committee itself and what it is attempting to do. The members are primarily from the larger countries that have large information activities. The present membership is as follows: Dr. Burton W. Adkinson (USA), Professor G. A. Boutry (France), Dr. H. Coblans (UK), Dr. H. T. Hookway (UK), Professor Dr. H. Kaiser (W. Germany), Professor Masao Kotani (Japan), Dr. P. Lázár (Hungary), Professor A. I. Mikhailov (USSR), M. P. Piganiol (France), Dr. F. A. Stafleu (Netherlands), Dr. C. Sherwin (USA), Dr. Harrison Brown (USA), Dr. A. Perez-Vitoria (France), and Professor N. B. Arutyunov (USSR).

Professor Arutyunov, who is on the Council of Ministers of the USSR, coordinates and administers the total scientific and technical information activities in his country. Professor Boutry is a physicist. Dr. Hookway heads the Office of Scientific and Technical Information in the Ministry of Education and Science. Professor Kaiser is a spectroscopist. Professor Kotani a bio-physicist. So you see there is representation by specialists in science information and by experts from various scientific disciplines.

In addition to this small working group called the Central Committee, a number of other people participate. In this connection an interesting "first" developed. It was the first time that representatives of OECD and its Eastern bloc counterpart, COMECON, had sat at a table to discuss problems of mutual interest. A fair number of representatives of other international organizations with large information activities also participated. These include groups such as EURATOM, CERN, IAEA, ILO, ISO, the ICSU Abstracting Board, and CODATA, which you will hear about from Professor Rossini. A number of people were afraid that this multiple representation from so many groups, including some from the East and West, would cause many political problems. (No problems developed.)

In addition, the Central Committee recognized the danger of becoming unrealistic and impractical in its planning and of getting into difficulties familiar to those engaged in the business of handling publications and in operating all the other mechanisms for the dissemination of information.

Thus, representatives of large abstracting and indexing services, and some publishers, were invited to join the Committee. Together, they make up an Advisory Panel of Operators of Large Systems. They attend the meetings, make comments, and hold separate meetings to consider agenda items that are coming up. They report to the Central Committee with suggestions for topics that ought to be investigated. A discussion has developed between those who have practical problems, and those who are taking a purely intellectual view with regard to how information activities should be organized on a world-wide basis.

The Committee's schedule calls for a report to be completed in 1970, and this is its prime purpose. The Committee is not a continuing group. It will take a look at problems worldwide and prepare suggestions for scientists, information people, librarians, as well as governmental and non-governmental organizations concerned with the broad problem. When the Committee submits its report, it is assumed that ICSU and UNESCO will see to it that any follow-on activities that are necessary at the international level will be organized.

At the present time a staff person is being sought to begin work with the Committee on the development of the report. Candidates for the position are being considered.

I should mention the current status of the financing of the operation. ICSU and UNESCO are planning further financial commitments to this work. UNESCO has recommended to its governing group that $150, 000 be set aside for UNISIST. ICSU itself has committed $15, 000 per year (which amount may be increased to $25, 000).

In summary, these are the areas with which this Committee is concerned and about which recommendations will be made:

(1) Improvement of the quality of science information, whether it is in primary publications, data, or other forms of

information. It will work with groups that are interested in the same objectives.

(2) Examination of the problem of analysis, reduction and compaction of information. In this area the CODATA program is of considerable interest to the Committee. The problem of reviews is being studied. Everybody says more reviews are needed despite the fact that thousands of reviews are being produced every year. The question is: Are they the right kind of reviews, and are they oriented toward groups who can use them?

(3) Improvement and coordination of large information systems. Many of the large programs are adopting automated procedures. What kind of recommendations, and what kind of organizational suggestions can be made to assist the development of these large systems, upon which many millions of dollars are being spent throughout the world? To illustrate the magnitude of this activity: U. S. Chemical Abstracts Service last year spent almost $14 million on its development program and operations. Systems of this magnitude are constantly being improved and need to be interconnected with other systems. What new mechanisms -- organizational, technical and otherwise -- must be developed to assist in getting a worldwide system that is more effective?

(4) Science information for the developing countries. How do we get information to them that they can use? We can send them tons of publications and all kinds of information, most of which may not be useful. The situation reminds me of the experience of the Atomic Energy Commission which made its publications available to most countries in the world. Several years ago someone from AEC visited the developing countries which had received these materials. He frequently found that the publications, catalogues, cards and indexes were still in the original containers. The recipients didn't know what to do with them. They didn't have the technical know-how, the money, or the organization to take care of them. These are the kinds of things regarding which UNISIST can make constructive suggestions.

How does a committee such as UNISIST operate in addition to having its regular meetings and a large advisory group? The approach has been to organize a series of working panels that meet several times between the main meetings. One panel already mentioned is concerned with the upgrading of the quality, the compression and analysis of information. This panel was chaired by Professor Kaiser of West Germany. The panel has made a constructive set of recommendations which are being studied to determine what further work should be done.

There is also a Panel on Bibliographic Standards. This panel is concerned with the question: "How can we standardize the citations and other bibliographic apparatus so that the information can be switched from one system to the other?"

What are the research problems and experiments that need to be undertaken in order to facilitate the development of systems that are compatible with one another? A panel is being established on the problem of language. How do we solve the problems of language and translingual transferability?

There is also a small panel attempting to determine how the large systems may assist the developing countries.

That, in brief, is the status of the work today: How we are going about the task with whom we are interacting. We hope we can meet our 1970 deadline for the submission of a report.

Consideration is being given to the possibility of convening in 1971 a conference of representatives of many different groups. They will be asked to review all the final recommendations and suggestions that we have developed under the auspices of UNISIST with the idea of analyzing and clarifying some of the recommendations. More importantly, they will advertise the need for better coordination and cooperation in the transfer of information of all kinds from one group to another and from one country to another.

Thank you.

DR. ASTIN: Thank you very much, Dr. Adkinson.

(A short recess was taken for coffee.)

DR. ASTIN: Gentlemen may we come to order, please?

We had planned for discussion at the conclusion of the formal papers this morning, and I hope that there will be time for that purpose when we get through the papers.

There is one more background paper before we hear from the representatives of the Advisory Board to the Office of Critical Tables. This paper will also be presented by Dr. Rossini.

One of the several hats that Professor Rossini wears is that of the U. S. National Member for CODATA. He currently serves as the President of CODATA. Dr. Rossini will report on this activity of the International Council of Scientific Unions. Fred?

WORLDWIDE ORGANIZATION FOR THE PREPARATION AND DISSEMINATION OF CRITICAL TABLES FOR SCIENCE AND TECHNOLOGY

By

Dr. Frederick D. Rossini, President
Committee on Data for Science and Technology of the International Council of Scientific Unions

There is little necessity today to justify our need for critical tables of numerical data for science and technology. Anyone who has engaged in the calculation of some problem in a given area of science or technology knows the extent of the frustration and of the loss of time resulting from inability to locate readily the value of a property critical to the calculation. Or, if a value is found, of not being at all sure of its reliability, and thus influencing the calculation in a most uncertain manner. When we take the average time lost by an individual scientist in this way in a year, and multiply it by the total number of scientists, we obtain a truly staggering figure of scientific man-days lost.

Apart from the time lost in searching for needed data, the problem of identifying reliability looms even larger. Records indicate that many enterprises have been started only to founder because of the unreliable nature of the data on which the decisions were based. There are many examples of such unfortunate failures, including several in recent years involving very large amounts of money.

Until about 30 years ago, most of the existing tables of data were prepared by scientists in their spare time, producing compilations in areas of their special interests. Then it became clear that the magnitude of the overall task of producing tables of data for science and technology far exceeded the capacity of a relatively few dedicated scientists working in their spare time.

We now see the quantity of scientific information doubling every 8 to 10 years. We note that there are of the order of 50,000 scientific journals in the world now. We estimate that 90 to 95 percent of all the scientists that have ever lived are living today, and that they are producing more than one million scientific and technical papers appearing each year in journals, bulletins, reports, and related media.

It is no longer possible for each individual scientist to review and appraise all of the numerical data in his field of interest appearing in original papers in the literature. He will not be able to review all of the relevant literature because of its magnitude; and he will usually not possess the expertise necessary to reduce and appraise the enormous amount of data to some understandable and useful meaning.

The solution to the problem of providing adequate data for science and technology is relatively simple. We need to arrange for the critical review and appraisal of the data in the literature, and the assembly of selected values of the properties into some useful form, by staffs of experts working full-time on the task. This work constitutes an intellectual task of high order. Though the work can be aided and expedited by automatic machines and high-speed computers, it can be performed effectively and efficiently only by having skilled scientists involved. We need to have more scientists dedicated to the work of critically reviewing and appraising the numerical data in the original scientific literature. To encourage this, we must see that the scientists engaged in this type of work are given appropriate high status in the scientific community, with corresponding compensation.

The numerical data which are to be reviewed and appraised for the benefit of science and technology are generated by observation and measurement, which operations constitute the backbone of science. The indexing, storing, and retrieval of the original papers is performed by information specialists skilled in their field. But the critical evaluation of the numerical data can be carried out only by highly trained scientific personnel with specialized knowledge of the material being evaluated.

Over the past several hundred years, man's capabilities for accuracy in measuring physical quantities has increased many fold, - in some cases as much as a million times better. Today, much of the numerical data appearing in the literature of the world is of very high accuracy and precision. In reviewing and appraising such data, it is important that all of the accuracy and precision be preserved in the transition from the original record to the final compilation. Further, where discord exists among data on the same properties, the appraiser must be able to derive from the detailed context of all the measurements that weighted value which is most likely to be near the true value.

With critical tables of reference data produced by experts of the highest competence, we can have efficient utilization of our scientific manpower in this regard. The end-using scientists in educational, governmental, and industrial organizations can then pursue the work of their respective missions, fortified with the knowledge that they have at their disposal essentially all of the existing numerical data in the literature reduced to some useable form of reference data. The number of man-days of scientific time that could be saved thereby in our laboratories would be enormous. But what is equally important, the numerical values available would be of much higher quality than could be produced by the sporadic effort of scientists primarily interested in other problems. This latter point is very important for our technology and industry today, where the precise control of temperature, pressure and other variables makes possible the conduct of industrial processes heretofore considered impossible. It is thus very important to have these numerical data for science and industry reviewed, appraised, correlated, and calculated by experts of the highest competence.

Let us now review briefly some of the international efforts on the compilation of data for science and technology.

The Landolt-Bornstein Tables, headquartered in Germany, first appeared in 1883 with an edition of 281 pages. The second, third, and fourth editions came out in the years 1894, 1905, and 1912. The fifth edition had eight volumes of 7457 pages over the years 1923 to 1936. The sixth edition had 24 books with about 24,000 pages, over the years 1950 to 1967. Because it is no longer practical for them to cover simultaneously all areas of science, the Landolt-Bornstein Tables have a new series of volumes, on specialized topics.

The Annual Tables of Constants, headquartered in France, had ten volumes appear over the years 1910 to 1930. From 1936 to 1945, there were forty installments, which covered the literature to 1939. Then a new title was given to this work, "Tables of Selected Constants", to cover specialized topics.

The Kay and Laby Tables of Physical and Chemical Constants, headquartered in England at the National Physical Laboratory, have appeared in one volume, running through 13 editions from 1911 to 1966.

The International Critical Tables, headquartered in the U. S. A., at the National Academy of Sciences-National Research Council, came out in the years 1926 to 1933, as one edition of eight volumes in 3, 819 pages. Details of this project were given in my earlier report at this meeting.

Also, as I reported earlier today, a number of other continuing data-compiling projects came into existence in the United States in the years 1938 to 1957. These projects together involved total expenditures of more than one million dollars per year, and covered physical, thermodynamic, thermochemical, thermophysical, nuclear, atomic, and all kinds of spectral data.

As described in earlier reports here today by Dr. Waddington and myself, a plan has been developed for handling the problem of data for science and technology in the United States which is comprised of the following components:

1. The Office of Critical Tables under the National Research Council.

2. The Office of Standard Reference Data under the National Bureau of Standards.

3. A number of privately supported data-compiling projects.

The plan envisages the following: that the NBS Office of Standard Reference Data will coordinate all work under government sponsorship and will provide funding for needed compilations; that the privately supported data-compiling projects will continue, and, hopefully, increase; and that the NRC Office of Critical Tables will coordinate and encourage the data-compiling activities in the private sector, will provide advisory services for the NBS Office of Standard Reference Data for the government sector, and will provide linkage with appropriate international organizations. It will seem, that given adequate funding from both the private sector and the government sector, this plan should be successful for the United States.

With this background, let us now have a look at the present international situation as regards data for science and technology.

In the spring of 1964, when it was abundantly clear that the problem of data for science and technology was an international one, it was suggested by the Office of Critical Tables through the Foreign Secretary of the Academy, that the International Council of Scientific Unions (or ICSU as it is called) take the lead in providing international coordination and guidance in this field. In June, 1964, ICSU established a Working Group, under Professor Harrison Brown of our National Academy of Sciences, to examine the problem. This Working Group met in December, 1964, at Washington, D. C., and formulated a recommendation that ICSU should establish a Committee in this field. In April, 1965, the recommendation was approved and the Working Group was requested to prepare a constitution and seek nomination for membership from unions and countries. This was done at a meeting in September 1965, at Frankfurt, Germany. In January, 1966, at Bombay, India, the General Assembly of ICSU, under Professor Sir Harold Thompson of the Royal Society in the U. K., approved the establishment of a Committee on Data for Science and Technology, or CODATA as it is called, together with a constitution and initial membership.

CODATA has the following assignments on a world-wide basis:

(1) To ascertain, through the Unions and appropriate National bodies, what data-compiling work is going on and what the needs are;

(2) To achieve coordination among, and provide guidance for, data compiling projects;

(3) To encourage support for data-compiling projects by appropriate private, governmental, and intergovernmental agencies;

(4) To encourage the use of internationally approved constants, units, and symbols, and, when desirable, uniform editorial policy and procedures;

(5) To produce a directory-survey of continuing data-compiling projects and related work;

(6) To encourage and coordinate research on new forms for preparing and distributing critically evaluated numerical data.

CODATA has held three annual meetings: In 1966, at Paris; in 1967, at Moscow; and in 1968, at Frankfurt.

The Bureau of CODATA has held six meetings in its three years of existence: One each in Paris, Moscow, London, and Enumclaw, Washington, U. S. A., and two in Frankfurt.

For its first two years, CODATA had its Central Office in Washington, D. C., with Guy Waddington as Director half-time. As of

July 1, 1968, the Central Office of CODATA was moved to Frankfurt, Germany, with Christoph Schafer as Director.

CODATA includes National Members, Union Members, Liaison Representatives, and Coopted Expert Members.

At present, we have seven National Members, Canada, France, Germany, Japan, United Kingdom, U. S. A., and U. S. S. R. Italy has accepted an invitation to become a National Member and the formalities are now underway. Several other countries have been extended invitations and are considering membership. At present we have ten Union Members as follows:

International Astronomical Union	IAU
International Geographical Union	IGU
International Union of Biological Sciences	IUBS
International Union of Crystallography	IUCr
International Union of Geodesy and Geophysics	IUGG
International Union of Geological Science	IUGS
International Union of Pure and Applied Biophysics	IUPAB
International Union of Pure and Applied Chemistry	IUPAC
International Union of Pure and Applied Physics	IUPAP
International Union of Theoretical and Applied Mechanics	IUTAM

CODATA has a number of Liaison Representatives, including one each from the following organizations: Federation of Astronomical and Geophysical Services (FAGS); ICSU Abstracting Board (IAB); International Atomic Energy Agency (IAEA); International Federation for Documentation (FID); Organization for Economic Cooperation and Development (OECD); World Meteorological Organization (WMO). Several others are also to be invited. In addition, CODATA regularly invites to its Annual Meetings Observers from the national government data program and from the National Committee for CODATA of the host country for the given meeting.

At the 1968 Annual Meeting, CODATA elected its first Coopted Expert Member, in the person of Guy Waddington, the former Director of CODATA.

The Bureau of CODATA has six Members: Myself of the United States as President; Sir Gordon Sutherland of the United Kingdom and Boris Vodar of France as Vice Presidents; Wilhelm Klemm of Germany as Secretary-Treasurer; and M. A. Styrikovich of the U. S. S. R. and Maseo Kotani of Japan as additional Elected Members.

National Committees for CODATA have been established in the U. S. A., the U. K., the U. S. S. R., Germany, Japan, and Canada. Italy is in the process of establishing a National Committee and each new country that becomes a National Member will also establish one.

The First International CODATA Conference, on the Generation, Collection, Evaluation, and Dissemination of Numerical Data for Science and Technology, was held at Arnoldshain (near Frankfurt), Germany, July 1 to 5, 1968, with near 100 experts in attendance from many different countries. This Conference, patterned after our Gordon Research Conferences, was so successful that the Second International CODATA Conference is planned to be held in 1970.

Much interest in the purposes and work of CODATA is becoming evident on all sides. The first tangible product of CODATA is now in process of preparation, - a Compendium-Survey-Directory of all the Projects in the World that are engaged in compiling numerical data for science and technology. We hope that this Compendium will be ready for distribution early in 1969. This Compendium will serve scientists and engineers the world over, informing them of what compilations are available, on what classes of compounds, on what properties, where available, and at what cost. The input to this important Compendium from the United States is provided by the Office of Critical Tables of our National Research Council.

For the purpose of improving international communication and understanding in the area of numerical data for science and technology, and of coordinating the work of experts in relevant areas, CODATA has established two Task Groups, is in the process of establishing a third, and has a fourth under consideration.

The first one established, the Task Group on Computer Use, has already held two meetings, one in Paris in 1967, and one in Washington, D. C., in 1968. This Task Group is making a survey of computer use in the storage, retrieval, and processing of numerical scientific data, and is studying the problem of compatibility of the different systems in use.

The second one, the Task Group on Key Values for Thermodynamics, has held one meeting in 1968, at Arnoldshain (near Frankfurt), Germany. This Task Group is to select a set of "key" substances for thermodynamic tables and to recommend values of properties to be assigned to them.

The third one, the Task Group on Fundamental Constants, is in process of formation. We hope the work of this Task Group will lead to an internationally approved set of fundamental numerical constants for science.

Under consideration by the Bureau of CODATA is a Task Group on Chemical Kinetics.

The cost of operating the Central Office of CODATA, amounting to about $60,000 per year, is covered by annual dues from the countries having national members. Our National Science Foundation supports the United States participation in CODATA. Unions and Countries are obliged to defray the cost of sending their representatives to the annual meetings of CODATA.

Broadly taken, the basic objectives of CODATA are to have compilations of critically evaluated numerical data for science and technology available in suitable forms on a world-wide basis, with the compilations satisfying the following requirements:

1. Covering all substances and all properties of interest to all sectors of the scientific and technical community.

2. Being fully self-consistent with all physical relations and with the internationally approved constants, units, symbols, and nomenclature.

3. Having an accepted standard order of arrangement, understood and usable at the bench by scientists in all countries, and produced in forms needed by the several sectors of the scientific and technical community, at the various levels.

4. Being produced by scientists of high capabilities, adequately compensated.

5. Being maintained up-to-date by revision at appropriate intervals.

6. Being adequately supported from governmental and private industrial sources.

7. Being readily available at reasonable cost in any part of the world scientific community.

In order to achieve these objectives, CODATA must provide the needed guidance according to a plan that will be freely acceptable to workers in the different fields of science in the different countries of the world. To be successful, any such plan should be practical and feasible in terms of existing intellectual and material resources. The plan should recognize all on-going compiling projects and their workers wherever they may be in the world and should coordinate and bring them together in an appropriate world-wide network.

One can envision a whole array of World Centers and Subcenters of Numerical Data for Science and Technology, one set for each small or large area of each field of science, all appropriately tied with a communication link to CODATA.

To see how such a system might operate, let us consider the hypothetical ideal case of XYZ data. It may happen that a given laboratory in a certain country will be the acknowledged world leader in compiling these XYZ data. In this case, the given laboratory may be identified by the experts in the given area as the World Center for XYZ data. All the other laboratories which are engaged in some compilation of XYZ data can be similarly identified as Subcenters for XYZ data, feeding their product into the World Center for XYZ data.

In many cases, it will not be possible to identify one laboratory as the acknowledged world leader in a given area of one field of science. In the given area of science, there may exist two or three or four laboratories of equal competence compiling data in the same general area. However, it is unlikely that each of these two or three or four laboratories will be working in precisely the same area of the given field of science. Usually, one will find that each laboratory has a concentration of interest somewhat different from the others. Accordingly one can subdivide the area of the given science into two or three or four parts, as necessary, and identify each of the two or three or four laboratories as a World Center for its particular variety of data. Each of these World Centers could have a set of Subcenters as previously mentioned.

In the overall plan envisioned here, the following points should govern:

1. The designation of the area of data to be covered by any one World Center and its allied Subcenters should involve considerable flexibility, to be expanded or contracted to fit existing projects in the most meaningful way. Existing realities should be recognized.

2. The designation for a given area of data, of the World Center and its Subcenters, or, in a special case, of several World Centers and their Subcenters, should be done by experts already engaged in compilation work in the given area. That is, the scientific decisions should be made by the appropriate scientists.

3. The information given in the CODATA Compendium, plus appropriate other information, may be used to determine given areas of data and to help designate the World Centers and Subcenters.

4. The World Centers and Subcenters should be distributed as far as possible over the scientific community of the world, with each country that has the necessary capabilities and resources sharing in the responsibility of providing these numerical data for science and technology.

5. The overall plan would be implemented gradually, stepwise, one area at a time, working forward slowly, and benefitting from experience in each case.

6. The plan would utilize only existing facilities and resources at the start, with no financial support being provided by CODATA for any compiling work on any project. The compiling projects linked into the plan would retain their existing financial support, their existing local direction, their existing local Advisory Committees, etc., maintaining essentially complete local autonomy for financial responsibility, scientific direction, and advisory services.

7. The plan would consist essentially in identifying World Centers and Subcenters among the compiling projects in given areas and tying these together with CODATA with an overlay of appropriate links in a world-wide communication system, including surface mail, air mail, telephone, radio, television, etc.

8. The Central Office of CODATA could become a repository for one set of all the data from each World Center and its allied

Subcenters, in whatever form it was created. All of the data so received by CODATA would have the original labels retained so that full credit is maintained for the original compilers.

9. CODATA could prepare and issue on a world-wide basis a current catalog of the data available from each World Center and its Subcenters, including adequate information for purchasers.

10. The Central Office of CODATA could receive orders from scientists anywhere in the world for data available anywhere in the world, and could arrange for shipment to be made to the purchaser directly from each compiling center. In this way, all of the world-wide data would become available to a given scientist with one communication and one payment. The cost for each kind of data would be fixed essentially by the creators, with advice from CODATA, with an appropriate discount being allowed CODATA to reimburse it for operating expenses for such distribution.

11. Whenever it was desirable, and agreeable to the creators of given lots of data, CODATA could prepare, by automatic means, special small handbooks of different sets of related data to serve the needs of bench scientists the world over.

12. The overall plan would also provide for special categories of Centers, involving handbooks and similar compilations.

13. CODATA would need funds only for the overlay of the communication system to link itself with all of the World Centers and Subcenters, and for the cost of providing the central information and order services.

14. As the plan develops and becomes successful, and when additional local funds are found, new compiling projects may be started in needed areas.

15. This plan appears to be compatible with the many suggestions and comments made on this subject at the First International CODATA Conference, indicating a desire to have a world-wide network with local autonomy which would provide for any scientist to learn easily what data are available, where, in what form, and at what cost, and to obtain the data by writing only to one place.

The foregoing plan will be under consideration by CODATA during the coming year.

DR. ASTIN: Thank you very much, Dr. Rossini.

Before hearing reports from Advisory Board members, there is time for a few questions addressed to any of the first three speakers.

DR. SCHULMAN: Dr. Rossini, the plan you have presented looks to me like a very detailed plan of operation. It is admirable. I am certain we can't digest the whole plan in a few minutes. However, it seems to be somewhat grandiose in its scope. I wonder how you feel it would work. For example, when there is a need for data, will people get that data from CODATA or from sources in the U. S.? I can see many problems, like developing countries wanting to specialize in certain areas. Are they to be excluded because they don't have standards of excellence now?

DR. ROSSINI: Well, there undoubtedly are problems, but let me answer the first question first.

The plan would simply involve CODATA sending an order received by them to Dr. Zwolinski in College Station, Texas, telling him to ship the requested sets of API Project 44 tables to whatever part of the world the original order came from.

DR. SCHULMAN: I thought you said it would be ordered directly from CODATA.

DR. ROSSINI: No. The Central Office of CODATA would receive an order from somewhere in the world for possibly 12 different kinds of data published in different places. CODATA would then be the servicing organization that would distribute these orders to where they have to go to be filled. The idea is to try to keep things much as they are at present but introducing some simple coordination which could be extremely useful at the international level.

Your second question was about the developing countries which do not now have work going on in these areas. I would think that these developing countries would be willing to accept that work done over here in established areas and would pick out some areas in new and growing fields of science that perhaps no one else or perhaps very few people are involved in. I think it would be possible by such means to get involved all people who sincerely desire to work on some part of the problem.

DR. ASTIN: Are there other questions?

DR. KAYAN: On the matter of unified presentations, is the matter of the metric unit system developing satisfactorily with special reference to the International System of units?

DR. ROSSINI: I am going to ask Dr. Waddington to answer that one.

DR. WADDINGTON: CODATA has considered at some length to what degree they could recommend the general adoption of the SI system of units by compilers the world over. This is a rather complex question, as you know, and in principle I think CODATA supports this proposition but they have not yet come out with a strong universal recommendation. However, the move is in that direction, and CODATA has been encouraged to note that the National Bureau of Standards is strongly encouraging the use of the SI within its own organization. The trend is now well established.

DR. KAYAN: Are thermodynamicists agreeable to dropping the calorie and the kilocalorie?

DR. WADDINGTON: I couldn't state that flatly, but I believe that the thermodynamicists have recognized that in time the calorie will pass away and be replaced by the joule. How long it will take, no one can predict.

DR. ASTIN: Dr. Brady, did you have something on this point?

DR. BRADY: The question of the general adoption of the SI by compilers is not an easy problem but we are doing what we can to encourage its use.

DR. ASTIN: Now we come to reports of Advisory Board Members who have been involved with a limited part of the data field, namely, "Numerical Data for Engineering and Technology." We will hear reports from four Members of the Board.

First, Dr. W. O. Taff, who is the Advisory Board Representative for the American Petroleum Institute, and is also chairman of the API Research Project 44, which compiles data on hydrocarbons. Dr. Taff.

THE PETROLEUM INDUSTRY

By

Dr. W. O. Taff, Advisory Board Representative
The American Petroleum Institute

MR. TAFF: Members of the Advisory Committee and Guests: It is a privilege to be invited to speak to you on this subject.

I am a representative of a major user group and really will speak to you from the point of view of a user rather than a compiler of information because that might be of most interest.

You will recognize that the petroleum industry, in the utilization of information, is not primarily interested in information on pure compounds. Neither is it generally interested in information of extremely high accuracy. It is interested in reliable data on multicomponent mixtures for use in the design of equipment, to assist in the development of new processes, and generally assist the petroleum industry to move forward in the effective and efficient manufacture of products that all of us use every day.

The most fruitful approach to developing the needed information is not self-defining. From an empirical point of view the realistic range of potential mixtures and property requirements is huge and the experimental problems formidable. From a more basic point of view the theory of mixtures is weak for many important properties and our ability to define compositions in terms of individual compounds or even in terms of important classes of compounds deteriorates rapidly above ca 200 °C.

As usual in a case like this we wind up working both sides of the street. The needs of the moment are real and cannot wait for the ultimate solution. The contemplation of what it would take to handle the entire problem by means of direct measurements on systems of interest drives you to pursue the more basic approach.

API has a Technical Data Book Project with which only a few of you will be familiar. Initiated in 1960 at Penn State under the direction of Prof. M. R. Fenske, this project has assembled a compendium of available and useful correlations covering a range of properties for mixtures. This was published in 1966 as "Technical Data Book -

Petroleum Refining". To date something over 2500 copies have been sold at $125/copy.

The API is committed to revisions and updating of this book. Such activity is now under way and a revised edition is likely to be printed in 1970. Holders of the book will have an opportunity to receive new information as it becomes available.

You will be familiar with API Research Project No. 44, "Data on Hydrocarbons and Related Compounds". This project was established in 1942 to provide a reliable source for needed physical and thermodynamic data on pure hydrocarbons and related derived compounds found in petroleum. As conceived, this project was expected to compile and publish tabular data selected from the literature by a process of critical evaluation and extended where possible and appropriate by correlation and calculation. It was also established that the tabulations were to be revised and updated as better data became available. The principal objective of this project may be stated as:

> Compile and make available for distribution critically selected data on the physical and thermodynamic properties of individual hydrocarbons and related compounds.

The project also has a second objective, added after initiation, to further serve the petroleum industry:

> Collect and make available in standard form for distribution spectra of hydrocarbons and related compounds which are useful for analytical purposes.

At the present time infrared, UV, Raman, mass and NMR spectra are collected and distributed. Most of these spectra come from within the industry and closely related groups.

Returning to the first objective of Research Project No. 44, you will recognize this to be the basic approach. Information of this type undergirds and permits expansion of information on mixtures.

The history of the project is interesting and is concerned with some of the principals here in this audience. Dr. Rossini was the first Director of Project 44. He continued as Director from 1942 until 1960. It is equally appropriate to recognize him not only as the first Director, but as the founder of this project, because he had a great deal to do with focusing the attention of influential men in the petroleum industry on the potential advantages of a cooperative project to assemble data on the properties of hydrocarbons since the information was obviously needed by everyone in the petroleum industry.

Dr. Rossini terminated his association with this project in 1960 when he moved from Carnegie Tech to Notre Dame. At that time, Dr. Zwolinski, who is also in the audience, became Director and continues to function in that capacity.

Physically, this project has had three homes. First it was at the National Bureau of Standards from '42 until '50. It moved with Dr. Rossini to Carnegie Tech and in 1961 it moved to Texas A&M, where it functions today as a significant part of the Thermodynamics Research Center.

There was also in existence in the period '47-'52 a subdivision of API Project 44 at the University of California under the direction of Dr. Pitzer. This program was active in the creation, compilation, and organization of useful thermodynamic data.

So much for the history of this project. What about its product?

The product of this project is basically tabular information of the type you have been hearing about today. The basic format is looseleaf to enable a continuous and effective updating by the process of substitution and addition.

The list of the physical properties that are included covers densities, boiling points, viscosities, refractive indices, critical properties, and many others. Thermodynamic properties include the free energy of formation, enthalpies of combustion and formation, entropies, heat capacities, and a goodly number of others.

The current catalogue of information includes data on 159 classes of hydrocarbons and related compounds in the sulfur, nitrogen, and oxygen series. The data is presented on over 2400 data sheets which are stored in six volumes. The separate numerical entries presently approach 410, 000. Supplements to this information are issued twice yearly in selected areas. It is obvious that it is not practical or needful to make a comprehensive review of all the information in any given year, or even in a period of years.

Some of the information in the most recent supplements concerns the physical properties of alkylnaphthalenes, vapor pressures and boiling points of alkanes and cyclo-alkanes, improved data on the enthalpies of combustion of alkanes, PVT information on methane, and a considerable amount of information on other properties of methane.

The product of API Project 44 has a wide distribution. At the present time there are over 1000 institutions and over 1200 separate recipients for various parts of its product. These people either subscribe and automatically receive supplements as they are issued, or they regularly purchase these supplements. The number of institutional recipients is roughly split 50-50 between industrial organizations and all others, including unversities, non-profit research groups, and so on. This overall group of recipients appears to be expanding in recent years at the rate of about 5 percent per year.

Financing of this project is of interest. Originally it was totally financed by the American Petroleum Institute with no real thought for the recovery of expenses. Of course, charges were made to profit-oriented organizations which did not contribute to the support of the project but a very large number of non-profit groups received the data sheets regularly on a gratis basis.

In the late 1950's, discussion began in the API as to whether or not the project should be placed on a self-sustaining basis. In mid-1965 it became an established objective of the project to become self-supporting. This objective will have been very closely approached this year at a budget level of about $95,000.

I will digress for a moment and say that the arguments pro and con for this move to a self-sustaining basis were many and diverse. To me, the most persuasive argument for seeking a self-sustaining basis was that it answers the question of the value of the project on a current and practical basis rather than axiomatically.

I have to disagree with Dr. Rossini's earlier comments about there no longer being any question about the justification for data compilation projects. I think on a philosophical basis we all agree with this. However, when you come to implementation you need to answer the questions of, "What is it worth to you?", "How much will you spend for a given data project?" The answers to these questions are not constant. Any policy groups concerned with such projects must give these questions continuing consideration.

In the industrial area the question of justification is likely to be re-examined at least as often as there is a turnover in the groups who control the money necessary to promote and support data projects. "Is the project justified?" "Don't tell me what it did for me yesterday, but what is it doing for me today, and what is it going to do for me tomorrow!"

There needs to be real consideration given to determining a mechanism by which value can be demonstrated. One of the best ways for value to be demonstrated is for the product of any project to be continually appearing on the desks of all the people who use such information in any given industry. That information needs to bear the name of the compiler and of the groups which sponsor the compilation. It needs to be distributed by a method and in a format that will make it useful to the groups who are concerned and not simply something that is tucked away in the library to be used only by those who are interpreting information for the benefit of their colleagues.

This was a digression. Now let me return to the main theme and conclude.

In arriving at a self-sustaining basis, we should not conclude that the American Petroleum Institute has severed its relationships with the project. At this point in time, rather, it means that the Institute underwrites or guarantees an operating budget at an agreed-on level. In this way the project is assured that its annual budget will be met.

The project continues to be guided as to directions in which its resources should be applied by an Advisory Committee which is appointed by the Institute. This advisory group also undertakes to comment on the effectiveness with which the project is meeting the needs of industry.

Now let me make a few additional comments about the Data Book Project to indicate to you the magnitude of this effort. This project was also conceived as a self-supporting project. I don't know whether it will ever reach that level or not. It has up to the present time cost about $360,000. A Technical Data Book has been produced and is for sale. About 2500 copies of the original 3000 printing have been sold at $125 a copy.

Overall costs of the project obviously exceed this income to the present time. This project, too, is on a continuing basis, and the Institute has made a commitment to continuously update this practical compilation of design information on a continuing basis.

The industry finds that there is not sufficient data in many areas for their needs so the industry does sponsor complementary data generating projects. One of those is located at the Bureau of Mines Laboratory at Bartlesville, Oklahoma, to produce new, accurate, thermodynamic data on hydrocarbons by experiment. There is a project located at Ohio State dealing with the critical properties of mixtures. There is a project at the C. F. Braun & Co. Laboratory to obtain enthalpy data on hydrocarbon mixtures, and there are others.

These activities are indications of the interest of the petroleum industry in having accurate information, of their need for accurate information, and of their willingness to pay for accurate information.

Dr. Bruno Zwolinski is here in the room and I would like to introduce him to you. (Prof. Zwolinski stands up). Bruno is the Director of the API 44 Data Project which is desribed in a blue brochure available at the registration desk.

DR. ASTIN: Thank you very much, Mr. Taff.

Most of the industrial laboratories of the United States are represented on the Industrial Research Institute. Dr. H. Heinemann is the IRI representative on the Advisory Board. Mr. Heinemann has had a long interest and association with data problems and will speak to us on IRI's views on this subject.

THE PROCESS INDUSTRIES

By

Dr. Heinz Heineman, Advisory Board Representative
For the Industrial Research Institute

DR. HEINEMANN: Mr. Chairman, Ladies and Gentlemen: My task here this morning has been made a great deal easier by Dr. Taff's lucid comments a little while ago. He has said much of what I intended to say to you about the need of industry, of the process industries in particular, for data and for data which need not be necessarily critically evaluated, but for which there should be some evidence of their accuracy and dependability.

Unlike the petroleum industry, which is a special part of the process industry, many of the other industries do not have projects of the type sponsored by the API that Dr. Taff has been describing. The result has been that throughout the years a large number of the chemical and chemical process industries have had to obtain data in their own research laboratories for projects which they had to design and for which data in compiled form were not available.

About two years ago when the Industrial Research Institute first appointed me as the representative to this committee, I had the opportunity of talking with Dr. Waddington and Dr. Van Olphen about the situation and pointed out to them that in my opinion there were large amounts of data available in industrial files which have not been made generally available to the profession as a whole. They, while agreeing, said "Well, do you know how many and is it really sizable?" Since then I have taken the opportunity of rather informally making a survey among IRI members, and I find that the great majority of chemical and petrochemical industry members have such data. I also find the general estimate that only about 25 to 35 or 40 percent of this data is ever published. The reason for the reluctance to publish data lies in the fact that the data are obtained for specific purposes related to a specific process and, therefore, are relatively incomplete from a general scientific point of view. The other reason is that very frequently these data are obtained for a process of proprietary nature and at the time they are being obtained, there is reluctance to make them generally available.

Of course, the need for restricting use of these data usually disappears in the course of a few years, and by that time there is no longer an interest in publishing them. It has, therefore, seemed to me that it would be very desirable to have available another data center. This center could act as a depository of data much in the way the American Documentation Institute functions for literature, and in which data that can be released by companies can be deposited without requiring a very careful summary and evaluation. It would be most important to have an index for this collection so that the data can be made available with the author's comments to anybody who is interested in them.

It has also seemed to me that the OCT or other similar organizations would need to coordinate this effort.

Thank you very much.

DR. ASTIN: Thank you very much, Dr. Heinemann for your report and interesting proposal.

Our next speaker is the Advisory Board representative for the American Society for Testing and Materials, Dr. W. L. Fink, who is also in charge of the ASTM X-Ray Powder Diffraction Data Collection.

Dr. Fink?

ANALYTICAL DATA FOR THE METALS INDUSTRY

By

Dr. W. L. Fink, Advisory Board Representative
For the American Society for Testing and Materials

DR. FINK: Advisory Board Members and Guests:

The subject for my talk that is given in the program is "Analytical Data for the Metals Industry," but my remarks will be restricted to ASTM's activity in this field with emphasis on the work done by the Joint Committee on Diffraction Data Standards.

ASTM's interest in the analytical field was initially in specifying methods of analysis. Description of methods has occupied a prominent place in the ASTM's Annual Book of Standards. But there has been a shift from wet methods of analysis to spectrographic and other instrumental methods. Interest grew steadily in having the data needed for instrumental analysis.

I shall discuss principally the publication through ASTM of powder patterns which are necessary for the identification of substances by diffraction methods. This service was initiated by ASTM's Subcommittee VI of E-4 in the late 30's. Then in 1941 ASTM joined with the National Research Council to form a Joint Committee to administer the work of this committee and to generate highly accurate patterns. The sponsorship of this committee has changed during the years. The present sponsors are ASTM, the American Crystallographic Association, the British Institute of Physics and the National Association of Corrosion Engineers.

From 1941, when the first set of powder pattern cards was issued, until 1950, financing was a serious problem. The committee was able to function only because of volunteer workers, free space and facilities at Penn State University, free publication and sales service by ASTM, and funds contributed by General Electric, Alcoa, Dow

Chemical, and other companies. However, as the sale of cards increased, the financial problem diminished, and the Joint Committee has gradually assumed more and more of the cost, until today it is self-supporting except that some patterns are donated and some overhead services are provided gratis.

Currently the committee is publishing about 2000 patterns per year. About 60 percent of these are gleaned from the literature or are donated. About 40 percent are produced by projects supported by the Joint Committee. There are such projects in Great Britain, Holland, Spain, Israel, and Japan, as well as in the United States.

The primary publication is on 3 by 5 cards or 4 by 6 keysort cards. During the first few years after the publication of particular groups of cards an intensive effort is made to find and correct any errors, and, to re-issue new improved cards. After that the material is also published in book form.

Now obviously, the use of these data for analysis will depend on some sort of search method which will allow one to locate the standard pattern that is to be compared with the unknown substance. Books are furnished with each set of cards. They index the patterns by the name of the substance and by the strong lines of the pattern. The first is known as the Davy or the alphabetical index, and the second is known as the Hanawalt Index or numerical listings. In this index, each pattern is listed three times -- in numerical order of the spacings corresponding with the strongest lines. Since some patterns cannot be found in these indices because the intensities are anomalous -- for instance, in the electron diffraction patterns -- another index known as the Fink Index is offered. This index uses the eight strongest lines and each pattern is entered eight times in numerical order of the spacing of these lines.

Another index with various uses, including the identification of minor phases, is the Matthews Index, which is a coordinate optical coincidence index. This has found considerable use.

There is also an alphabetical index which is an improvement over the Davy Index and will probably be substituted for it in the near future. This is a key-word-in-context index very similar to the American Chemical Society Index.

The most recently adopted search procedure is a computer method developed by Dr. Johnson and the late Dr. Vann at Penn State.

The Joint Committee leases the file on tape with appropriate search programs. Moreover, for those who do not have a computer, the General Electric Company and ASTM have just set up a remote access to the ASTM powder diffraction data, which gives anyone in the United States access to the ASTM file in the GE 635 computer system through a terminal in his own laboratory and normal telephone lines.

I will mention three new developments which have not quite reached the stage of general sale.

The whole file consisting of approximately 16,400 cards, has been condensed by putting it on microfiche, so that 137 microfiche, which can be held easily in one hand, contains the whole file. It is hoped that the Joint Committee will be able to offer this form for lease early next year.

An improvement on the present Fink Index has been tried out on a very limited scale and looks promising. It is a graphical index, using the same eight strongest lines that are used in the present Fink Index. The graphical index is much more rapid than the numeric index, and besides, it locates solid solutions readily. The other index books that I have mentioned often fail to find solid solutions. The principal hurdle to offering this index is the high publication cost. We have hopes, however, that this can be decreased to a reasonable level by new high-speed photo composition machines, when they become available to the committee.

Dr. Visser, of our Holland project, is working on a further improvement of the Fink graphical index. Holograms of the graphical eight-line index are prepared and are compared optically with a transparency of the unknown pattern. Initial work looks very encouraging. Much more work needs to be done to develop it to a useful stage, but Dr. Visser believes that the method will, in time, be relatively cheap and will be as fast as computer search.

I will now mention very briefly some other ASTM analytical data activities.

Until recently, various ASTM technical committees have worked almost completely independently in various fields -- E-2 on emission spectoscopy, E-13 on molecular spectroscopy, E-14 on mass spectroscopy, and E-19 on chromatography. Very recently, the editorial work of all these committees, and also the Joint Committee that I discussed, have been merged into a Division of Atomic and Molecular

Data. Dr. Simard who has been the manager of the Diffraction Section, is now the manager of this new division.

Work is underway to revise, enlarge and update the publication of Committee E-2 on X-ray emission line and wave lengths and 2Θ tables.

In Committee E-19, a compilation of gas chromatographic data has recently been published, and an enlarged publication on this subject is contemplated in the near future. The data are also available on punch cards. The ultimate aim is to produce an index to all the reliable published data on liquid and gas chromotgraphy for the separation and the identification of materials.

Early in 1969 there will be published a new index of mass spectra by Committee E-14. The old index is now out of print and out of date. The spectra will be indexed by molecular weights and peaks, and will be available on tape for search by an IBM 360 computer. It will probably also be available on the coordinate index using ter-matrex cards.

Committee E-13 is continuously publishing indices to absorption spectra of chemical compounds. The basic index consists of IBM cards which are available for purchase. To date there are more than 90,000 cards in the infrared index, and more than 25,000 in the ultraviolet and visible. From these cards index books are prepared, one, indexing all infrared cards by serial number, another indexing all infrared cards by formula, and the third indexing all ultraviolet and visible cards by formula, and a fourth indexing all ultraviolet and visible cards by serial numbers.

Tapes have also been prepared from these cards, and search programs are furnished with the tapes. The most recent development in computer searching for infrared spectra is the ASTM-Dow Sirch System. It is an improved computer search procedure for an IBM 1130 which is a low-cost computer. The coding is very simple. It includes wave lengths or wave numbers and 32 codes for other physical data. The search system was developed by Dr. Erley of the Dow Chemical Company.

The entire file and search program are on three memory discs which can be searched at the rate of about 1000 spectra a second. The output is ASTM serial numbers, which can be looked up in the index book.

In the near future, we will start work on the inclusion of ACS registry numbers for all compounds in the data publication of the ASTM committees. This should be a big step in coordinating ASTM and ACS data projects.

Now, this account has necessarily been very brief. I hope it may give you a picture of a going activity that is supplying needed analytical data to industry.

Thank you very much.

DR. ASTIN: Thank you very much, Dr. Fink.

(Recess for lunch - - 12:00 noon to 1:00 p.m.)

AFTERNOON SESSION

Chairman: Professor Frederick D. Rossini

DR. ROSSINI: We will start our afternoon session a little early in order to conserve time. We will begin with Item (d) of the last part of the morning program. I now call on Dr. Taylor Lyman, the Advisory Board representative for the American Society for Metals, who will share the reporting on mechanical properties of metals with Frank Speight, speaking for the Metal Properties Council. Dr. Lyman?

MECHANICAL PROPERTIES DATA FOR THE METALS INDUSTRY

By

Dr. Taylor Lyman, Advisory Board Representative
For The American Society For Metals

DR. LYMAN: The project that I have to report to you, Members and guests, concerns the publication of mechanical property data that the American Society for Metals has been responsible for in Volume 1 of the Metals Handbook.

This handbook project, which has been a continuing one since 1923, is primarily a publishing project, with strong elements of data collection. The mechanical properties that we have published in Volume 1 of the 8th Edition of the Metals Handbook are certainly not critical data, but they do represent an extensive collection effort.

The data in this volume were contributed by more than 1000 people who were organized largely into committees to treat various topics.

Perhaps one item of special interest in connection with these mechanical property data is that we did recognize uncertainties in the mechanical properties of many alloys by publishing histograms (statistical distribution of property values). We had nearly 1000 histograms in this book concerning mechanical data.

The scale of the handbook effort is of the order of $700, 000 a year, of which about one-third is for technical staff and editorial work, and the rest for cost of goods, distribution, and various administrative expenses.

We have found in general the problem that Mr. Heinemann mentioned. For a period of time the data are considered proprietary by the companies and then they become obsolescent. But we have also found that there is a very short period between the time they are proprietary and the time they are obsolescent. If you can get the data at just that moment and publish them then there seems to be a continuing demand. The best evidence of this fact is the continuing sales history of the old International Critical Tables. Our own Volume 1 that we have in circulation now has sold a total of 76, 000 copies in a period of seven years, and it continues to sell well. So it is possible for some of these programs that we have been talking about today to be self-sustaining on the basis of their own sales of products. At least that has been our experience, although it took a number of years to reach that point.

Perhaps the most interesting project that is going on right now in the field of mechanical property data is the work of the Metal Properties Council. Because I am not closely associated with this program myself, I have asked Frank Speight, of the Engineers' Joint Council to describe it to you. Frank is here and has kindly consented to tell you about the Metal Properties Council.

METAL PROPERTIES COUNCIL

By

Frank Speight, Engineers' Joint Council

MR. SPEIGHT: Thank you, Taylor.

Dr. Astin, Ladies and Gentlemen: I am not with The Metal Properties Council (MPC) but serve on the staff of the Engineers' Joint Council. I am speaking for Adolph Schaefer, Director of the MPC, who had a conflict. He is also the chairman of Committee A-1 on Steel of ASTM, which meets this week. The Committee develops product specifications for steel as well as many of the test methods that the Metal Properties Council uses for reporting data on the properties of metals.

The Metal Properties Council was established about three years ago. It is jointly sponsored by the Engineering Foundation and by three technical societies -- American Society for Testing and Materials, American Society of Mechanical Engineers, and American Society for Metals. It grew out of the work of the Joint Committee on Effect of Temperature on the Properties of Metals which was organized in 1925. It has been active for more than 40 years under the joint sponsorship of ASTM and ASME.

ASTM has the materials property interest, the people who know materials. ASME has the people who are concerned with engineering designs, with the development of codes and standards, and with the data needs for codes and standards. The Joint Committee on the Effect of Temperature on the Properties of Metals has over a long period of time developed data on the properties of metals principally for use in developing the boiler and pressure vessel codes of ASME.

The work in this area got to the point where it was too much for a volunteer-type operation, which the Joint Committee was, and they also wanted to establish it at a high level in the engineering community. The Engineering Foundation provided seed money to establish the Metal Properties Council under the sponsorship of the three societies I mentioned.

It has two principal operating groups. The Board of Directors is business-oriented, and the Technical Advisory Committee is oriented toward the technical needs of the industry. It has these four points as its major goals: To identify the major needs for reliable data on the engineering properties of metals and alloys -- and here I might digress for just a moment on "engineering properties." By "properties" we mean what Guy Waddington said when he referred to them as "arbitrary parameters," because these properties are based on standard methods of test.

The second goal is to evolve plans and to conduct programs for collecting, generating and evaluating such data so that it may be useful, this critical part of it.

The third goal is to make these data available properly by reports, publications, correspondence, and other means. The reports and publications are handled by the Metal Properties' Council's sponsoring societies, ASTM, ASME and ASM.

Fourth in the goals is to assure nonduplication of effort by keeping abreast of current national and international developments in the fields of metals engineering research.

I might say that the output of the Metals Properties Council, the data on properties of metals, is of considerable interest to the industries that were just mentioned by earlier speakers; the petroleum industry uses the codes and standards based upon MPC data for construction of their process equipment, piping, and so forth; and similarly the chemical industry and all industries that use pressure vessels and piping, are dependent upon the data that is turned out by the Metal Properties Council by using the codes and standards based upon the data.

There are six projects currently underway by the Council, and I will review them very briefly.

In the boiler and pressure vessel technology field, the Council has collected extensive data on carbon and alloy steels, which are being analyzed for subsequent publication. An evaluation of stainless steel data is being published by ASTM. Extensive studies have been instituted for the evaluation of present parametric methods as applied to elevated temperature creep testing. It is possible that an entirely new parametric approach may be developed.

The Council is also studying creep and stress rupture properties of aluminum alloys.

The second item is a two-year program to test high-temperature performance of quenched and tempered chrome, molybdenum and steel plate.

The third item: Determining characteristics of metal and special alloys for power generation, petroleum, chemical process equipment in sophisticated low-cycle fatigue. Now, the term "low-cycle fatique" should have some explanation. We must always explain words or we don't communicate. "Low-cycle fatigue" occurs, for example, when a power plant is started up and then it is shut down and then it is started up, this is low-cycle, but it is fatigue, because the equipment goes through the cycle of temperature and stress, and this influences how long these metals will last in service under the extreme conditions of temperature and pressure.

The fourth program that is going on is to determine the effect of loading rate on metal strength. Fatigue tests, for example, are generally run at high repetitive loading rate, but if you run a more or less static tensile test, the speed with which you pull the bar is important in the number you get in the value for the test method, so the Council is studying the effect of loading rate on metal strength values resulting from the tests.

Number five in the program involves testing for the relaxation characteristics of metals.

The sixth one is on determining the effects of radiation on the properties of metals, and this has particular application in the nuclear power field.

These are the major programs. There is research work going on in the Joint Committee, ASTM, and ASME also sponsored by the Metal Properties Council. They are determinig the properties of super-alloys, properties at very low temperatures, notch effects, and other significant properties.

There are pieces of descriptive literature at the registration desk. One of them, issued by ASME, is "Analysis of Data From Symposium on Heat Treated Steel for Elevated Temperature Service." Another is "Elevated Temperature Properties of Selected Super-Alloys." It is of particular interest. The work was done in cooperation with the Defense Metals Information Center at Battelle, which was one of the joint sponsors for the project. The method of collecting data from industry is of interest. The Council has established a standard form for reporting data on properties of metals which is distributed widely to companies in the industry. The companies then identify their products that fit the particular survey, and they fill in not only the composition, the characteristics of the particular alloy, but also its properties.

This is the sort of mechanism mentioned by Dr. Heinemann this morning that is needed to collect data in company files that alone are not very useful, but in combination with other comparable data are useful. The Metal Properties Council is quite active in collecting data in this way.

The Council operates on a rather low administrative budget of about $35,000 though the total budget for testing and analysis of data is some $300,000 annually. The funds are obtained from industry by periodic solicitation. (Further information about the Metal Properties Council and its program are contained in Annex I, pp. 144-147).

DR. ROSSINI: Thank you. Thank you very much Mr. Speight and Dr. Lyman.

Now we have time for a few questions or comments should there by any. Dr. Brady?

DR. BRADY: This morning Dr. Heinemann mentioned the possibility of a depository for company or industrial data. I wonder if there has been any consideration given to such a depository in the system that the Tripartite Committee is studying for engineering information systems.

MR. SPEIGHT: One of the other hats I wear is as secretary of the Tripartite Committee, which is composed of representatives ofthe Engineers Joint Council, Engineering Index, and United Engineering Trustees. There is currently being conducted a study by Battelle Memorial Institute for the Tripartite Committee and supported by the National Science Foundation which is intended to develop an engineered plan for a limited Engineering Information and Data System to be operated under the general auspices of the Engineering Societies. The study is expected to be completed by the middle of 1969. I can't answer the specific question as to whether or not the results of this study will include a recommendation establishing such a depository, but it seems like a reasonable recommendation.

DR. ROSSINI: If there are no additional questions now, perhaps later in the afternoon there will be time for discussion. Meanwhile, we will proceed directly to the program for the afternoon session. I first call on Dr. Allen Astin, the Director of the National Bureau of Standards, who has had an intimate connection for a long time with the critical tables problem, since he was, as I mentioned this morning, chairman of the old NRC Committee on Tables of Constants. He was also the first chairman of the Executive Committee of the Office of Critical Tables and served from its establishment in 1955 until 1963, when by request he became an ex-officio member of that committee because the National Standard Reference Data Program had been established at the National Bureau of Standards.

Dr. Astin?

INTRODUCTORY REMARKS ON THE NATIONAL STANDARD REFERENCE DATA PROGRAM

By

Dr. A. V. Astin, Director, National Bureau of Standards

DR. ASTIN: Thank you very much, Dr. Rossini.

The remainder of the afternoon program is devoted to reports on the activities and goals of the National Standard Reference Data System as operated by the National Bureau of Standards. It is my purpose to give brief introductory remarks for the presentations which will be made by Dr. Brady and his colleagues at NBS who are all deeply involved in these activities.

The National Standard Reference Data System has its origins in the work of the Office of Critical Tables and its Executive Committee in the National Research Council. It was about eight years ago that the Executive Committee came to the conclusion that success in initiating the new data compilation activities that were necessary to meet the growing needs of scientists and engineers throughout the country would require a significant Government contribution. The matter was then considered in depth by the Federal Council for Science and Technology and as a result of the Council's deliberations there was established a National Standard Reference Data System, with responsibility for operating this system being assigned by the President's Office of Science and Technology to the National Bureau of Standards.

The purpose of the system is to provide a central, coordinating point for the data compilation activities of the Federal Government; to provide information as to what data are available through the operation of a central national file; to seek to acquire funds to establish new compilation programs; and to establish standards for standard reference data.

Because of this assignment, the acquisition of funds for the implementation of the program received the highest priority in the fund acquisition efforts by the National Bureau of Standards. We have not, however, been nearly as successful in this effort as we had hoped, but we are still optimistic.

Added support was given to the program by action of the Congress this past summer when it passed legislation [1] which endorsed the essential objectives delegated to us by the Federal Council for Science and Technology, and assigned clearly to the Secretary of Commerce the responsibility for operating a National Standard Reference Data System.

Among other things we derive one advantage from this legislation in that the House Science and Astronautics Committee will provide annual authorization hearings for the program, and thereby we hope to develop support and interest in the program on a broader scale in the Congress than just in the Appropriations Committee.

The bill also gave us another additional important authority in that it permits us to copyright or secure copyright exceptions for standard reference data, in the hope that we will have a mechanism through sale of publications and services for recouping part of the costs of the operation of the system. Dr. Taff's report earlier in this meeting on the success of the American Petroleum Institute Research Project 44 in becoming self-supporting through sale of its publications and services is very encouraging to us. Perhaps with the new authority for the Standard Reference Data System we can augment the resources available to the program more rapidly than through direct appropriations alone.

In operating the program, the National Bureau of Standards looks to the National Research Council of the National Academy of Sciences - National Academy of Engineering, for advice and guidance in setting priorities and in enlisting the support and cooperation of the Nation's scientific and engineering community in developing and disseminating standard reference data. I believe that the National Bureau of Standards, in terms of its relative size, makes more use of the National Academy for advisory services than most other Government agencies, and certainly we will look to the Academy-Research Council

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

for this type of help and guidance in the future.

In this connection the Advisory Board of the Office of Critical Tables will, I hope, be a major source of input to our program. I do not expect that it is reasonable in a large meeting such as this to get detailed suggestions as to how we might better improve our operations, but certainly this meeting here today gives us an opportunity to outline to you what we are doing and what some of the problems are. I hope each member of the Advisory Board will personally interest himself in the program and send us his comments from time to time as you or others in your organizations get ideas about how the program can be made more useful and carried out better.

There is one related comment that I want to mention, particularly since Dr. Waddington in his paper this morning made reference to the importance of identifying the particular fundamental physical constants or measurement systems that might be involved in all data compilation programs.

There were a number of actions of significance to data compilers taken by the International Committee on Weights and Measures last month (October 1968) at its annual meeting in Paris. Probably the most important was the decision to promulgate on the first of January 1969 a new revision of the International Practical Temperature Scale. This new scale will extend below the oxygen point to the hydrogen point, and will also specify revised methods of interpolating between all the fixed points on the scale. In addition, the Committee changed the value of the volt by 11 parts in a million. This action was the result of a number of international comparisons. The Committee also adopted a new value for the gyromagnetic ratio of the proton and adopted a new value for the acceleration of gravity, changing the old Potsdam value by 14 parts in a million.

All of these activities are of significance to data compilers. They will be summarized in an early issue of the Technical News Bulletin of the National Bureau of Standards.

The details of the operation of our National Standard Reference Data Program will be presented by Dr. Brady and his colleagues.

I would like to close by thanking each of you for your interest in coming here, and urge again that your interest not end with this meeting. Please keep in touch with us, passing on your suggestions from time to time.

Thank you very much.

DR. ROSSINI: Thank you very much, Dr. Astin.

I now call on Dr. Edward L. Brady, the Director of the Office of Standard Reference Data at the National Bureau of Standards, who has been in charge of this program since its inception in 1963. Dr. Brady?

PROGRAM AND PLANS

By

Dr. Edward L. Brady, Director
Office of Standard Reference Data, National Bureau of Standards

DR. BRADY: Thank you, Dr. Rossini.

People have been compiling and storing quantitative data on properties for a long time. Figure 1 is a fairly early example of a data compilation. This one might well be called "The Pre-Druid Astronomical and Solar Forecasting Data Center."

Similarly, there is nothing new about NBS involvement in data compilation activities; data compilations have been among the most valuable NBS products throughout its history. An important example is Circular 500, "Selected Values of Chemical Thermodynamic Properties", which has been used as a definitive source of reference data by thermodynamicists since 1952. Another example is the atomic energy level compilations of Dr. Charlotte Moore Sitterly, which have been used by astrophysicists, theoreticians, and analytical chemists for many years. Several other activities could be mentioned that were in existence long before the National Standard Reference Data System was established or even dreamed of.

These activities are in keeping with the National Bureau of Standards' mission of looking after the good health of the "National Measurement System." The concept of the National Measurement System is basic to a relatively new description of the mission of NBS. I will describe it briefly since most of this audience probably is not familiar with the concept. I want to emphasize that we do not talk about a new mission for NBS. We just have a relatively new description of the mission that NBS has had since it was created. In this

formulation, the National Measurement System is regarded as the total complex of activities within the United States that lead to meaningful quantitative measurements of properties of substances and systems. Within this complex NBS has a responsibility to ensure that adequate measurement tools are available to the U. S. technical community. This means that NBS must take appropriate steps to assure that the nation possesses the technical ability to measure mass, length, time, and temperature as accurately and precisely as needed by American science and technology. It also means that NBS must take appropriate steps to ensure the ability to measure the derived quantities -- for example, ampere, capacitance, emissivity -- as accurately and precisely as necessary. Going on from the derived quantities, the NBS mission includes the responsibility to assure that measurement tools are available to measure the properties of substances -- such as crystallographic structures, thermodynamic functions, atomic collision cross sections, etc. -- as accurately and precisely as possible.

At this meeting, it is not appropriate to attempt to describe in detail the anatomy of the National Measurement System. I would like to refer you to a description by Dr. Robert D. Huntoon that appeared in SCIENCE magazine in the issue of October 6, 1967. I'll be happy to send a reprint to anyone who requests it.

And now I turn to the relevance of the mission of the National Standard Reference Data System to the National Measurement System. The results of property measurements are part of the storehouse of information included within the National Measurement System. If these results are usable by someone else, the measurement system need not make another measurement. The efficiency of the System is increased. NBS then, as the promotor of the good health of the National Measurement System, has a responsibility to ensure that these useful results are adequately available to the technical community of the United States. That is what the National Standard Reference Data System is all about. We are endeavoring to organize and coordinate a continuing comprehensive program of collecting and reviewing the world's literature, extracting and evaluating quantitative data on properties, and compiling and disseminating these results for use by scientists and engineers.

However, ouf experience so far has shown that the contributions made by data analysis centers to other aspects of the national Measurement System are also of vital importance. These contributions consist of pointing out the limitations and uncertainties and experimental techniques, of identifying discrepancies in experimental results, and of pointing out new or more precise measurements that need to be made. That is, the data centers make an important contribution to the guidance of experimental work in the fields in which they are active.

As already pointed out in an earlier talk this morning, the NSRDS dates from 1963. Its establishment arose from the recognition by the Federal Council for Science and Technology that a systematic effort of this sort was needed. The National Bureau of Standards was requested to assume the responsibilities shown in Figure 2. This FCST action was reinforced last summer by special legislation passed by the United States Congress, directing the Secretary of Commerce to provide compilations of critically evaluated data as needed by the technical community of the United States and providing certain other authorizations that enhance the ability of the National Bureau of Standards to carry out the program.

In developing the program of the Standard Reference Data System, three basic policies were established that have determined the structure of the activity. These three policies are the following: 1) the effort must be continuous, rather than start-and-stop; 2) only specialists in the subject matter are able to evaluate data adequately; and 3) financial remuneration for this type of program should be comparable to that for any other sophisticated professional activity. These basic policies have led to the organizational policies shown in Figure 3. These policies have guided our actions throughout the development of the program.

So far I have set only very broad limits of the scope of our activities by talking about quantitative measurements of properties of substances. However, it is not practical for us to attempt to be concerned with all properties of all substances and combinations of substances. For the present and foreseeable future, we have limited the scope of the program to "quantitative information relating to a property of a definable substance or system." In practice, this means that if the property under consideration is a sensitive function of impurity or structural features which are unknown, the property is not considered within our scope. Also, if the substance is a complex and variable mixture, such as concrete, most commercial alloys, or most organic polymers, it also is considered not within the scope of the system. We realize that adoption of this scope excludes from our program some of the most important properties and substances of interest to technology and commerce. We hope that it will eventually be possible for us, or for someone else, to develop a systematic program to handle these types of data.

Figure 2

RESPONSIBILITY OF NBS-OFFICE OF STANDARD REFERENCE DATA

1. TO PROMOTE THE GENERAL OBJECTIVE

2. TO COORDINATE RELATED WORK

3. TO ESTABLISH STANDARDS OF QUALITY

4. TO OPERATE A NATIONAL STANDARD REFERENCE DATA CENTER AT NBS

5. TO ESTABLISH STANDARDS OF METHODOLOGY AND OTHER FUNCTIONS

Figure 3

ORGANIZATION

1. LOCATION WITHIN LABORATORY OR OTHER TECHNICAL COMPONENT

2. PROJECT TO BE LOCATED WHERE DEMONSTRATED COMPETENCE IN SUBJECT ALREADY EXISTS

3. DIRECT SUPERVISION OF PROJECTS BY LOCAL MANAGEMENT

4. PROJECTS TO BE INITIATED WITH ASSUMPTION THEY ARE TO BE LONG-TERM RATHER THAN ONE-SHOT

5. SUBJECT SPECIALISTS TO BE PART-TIME EVALUATORS AND COMPILERS

6. ADVISORY PANEL OF SUBJECT SPECIALISTS AND USERS TO BE ESTABLISHED

In each program category, we are endeavoring to develop a coordinated network of continuing data analysis centers. In Figure 4 thereis showna representation of the sequence of activities followed within a data center, and types of products that result from these activities. The first step in any center is to select and collect relevant material from the vast quantity of world literature produced each year. This material is then indexed in an appropriate way and stored for rapid retrieval. The next step is to extract from this stored material the quantitative data to be evaluated plus any additional information required -- such as experimental techniques, statistical treatment given to the data, and other relevant information. This is then followed by a critical evaluation of the data, a subject for for an all-day discussion in itself. I will not attempt at this time to go into detail about what we mean by critical evaluation.

The right hand column of Figure 4, indicates the type of product produced as a result of the activities just described. Each of the data centers associated with the Standard Reference Data program must carry on the evaluation process; the other activities listed are necessary but not sufficient. Initially in our program, heaviest emphasis was placed on the production of compilations and critical reviews, but recently we have found it necessary and desirable to place emphasis on criteria and recommendations. Criteria may be of three types: a) for making measurements in the laboratory, b) for reporting results in the literature, or c) for evaluating results already reported.

In this presentation, I have tried to outline the background and philosophy of operation of the National Standard Reference Data System. For the balance of the afternoon, the speakers that follow me will present to you some detail about what is actually going on in each of our program elements. The following speakers are members of the staff of the Office of Standard Reference Data with one exception, Dr. Lee Kieffer. Dr. Kieffer is in charge of the center on Atomic Collision Processes of the Joint Institute for Astrophysics at the University of Colorado. We have asked him to talk this afternoon because we consider his center to be an example of the objective we try to promote of achieving good coupling between the experimental program in the laboratory and the work of the data center itself.

I want to thank you for coming here today to listen to our program. We welcome comments and inquiries from each of you and we hope that you will not hesitate to write or call us.

Figure 4

INFORMATION ANALYSIS CENTERS

ACTIVITIES AND PRODUCTS

Activity		Product
COLLECTION ↓	→	BIBLIOGRAPHY
INDEXING ↓	→	INDEXED BIBLIOGRAPHY
EXTRACTION ↓	→	DESCRIPTIVE REVIEW UNCRITICAL DATA COMPILATION
EVALUATION	→	CRITICAL REVIEW CRITICAL DATA COMPILATION CRITERIA RECOMMENDATIONS SOLUTION TO PROBLEMS CORRELATIONS

Within the National Bureau of Standards, the Office of Standard Reference Data has been established as one of the components of the Institute for Basic Standards. The Office of Standard Reference Data is for program management purposes only; only in very special circumstances are compilations produced by the staff of the Office of Standard Reference Data. The great majority of evaluation and compilation projects are conducted within the experimental divisions of NBS, in other national laboratories operated by other agencies of the United States Government, in universities, or other laboratories.

The NBS Office of Standard Reference Data has responsibility for the following three functions: 1) to plan, coordinate, and monitor the program of a network of data analysis centers that produce critical reviews, data compilations, and other products needed by the technical community; 2) to develop methods of improving information processing techniques within data centers through use of computers and other new technology; 3) to make the results of the program as accessible as possible to the entire technical community of the United States. Up to the present, our primary emphasis has been on the first function, into which the largest portion of our available resources has gone.

For internal management purposes, we have established seven broad subprograms of data compilation activities. These are concerned with nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, properties of chemically reacting systems, surface and colloid properties, and mechanical properties. Most emphasis in our funding has been placed on the two categories of atomic and molecular, and thermodynamic properties. The Atomic Energy Commission has had an extensive program to compile nuclear property data throughout its history. The Department of Defense and NASA sponsor useful and effective programs in a number of areas within the scope of the NSRDS, as well as numerous others outside the scope at the present time.

In each category, an advisory panel has been established primarily under the sponsorship of the National Academy of Sciences-National Academy of Engineering. The panels are formed as subcommittees of the general Advisory Committee for the Office of Standard Reference Data, identical in membership with the Executive Committee of the Office of Critical Tables under the chairmanship of Professor Frederick Rossini. The recommendations and comments of these advisory panels have been of enormous importance in providing guidance to the activities of the program.

DR. ROSSINI: We have some time for general questions to Dr. Brady about this program before the specific reports on it are given to you by his colleagues. Perhaps you will think of some later. Meanwhile, I will ask Dr. Brady if he will take the chair and introduce his associates.

DR. BRADY: As I mentioned, the two areas of principal emphasis within our program categories have been those of atomic and molecular properties and thermodynamic and transport properties. Those are the first two subjects that we wish to present to you today.

The man who will describe the activities in the atomic and molecular property category is Dr. Stephen A. Rossmassler, who is on the personnel rolls of the Office of Standard Reference Data, but for some time in the future will be on assignment with the President's Office of Science and Technology in the Executive Office Building here in Washington, working with the group on the problems of handling scientific and technological information within the United States. Dr. Rossmassler?

ATOMIC AND MOLECULAR PROPERTIES

By

Dr. S. A. Rossmassler

DR. ROSSMASSLER: Thank you, Ed.

The program for data compilation of atomic and molecular properties got underway early in 1964, which was about the time that the Standard Reference Data System began to function as an entity. We saw three immediate needs in starting this program: First, to define the scope; second, to identify ongoing activities inside and outside the National Bureau of Standards; and third, to initiate new projects in areas of high priority.

In order to begin this program, we did feel that we had to put some boundaries on the broad area of atomic and molecular properties. As the first of several successive approximations, we decided that we would concern ourselves with properties characteristic of individual atoms and molecules rather than of any specific state of aggregation. This means, of course, that topics like crystallography are not included as atomic and molecular data.

We used this definition for planning, for identifying ongoing projects, for starting several new projects that we thought should be initiated immediately. On the basis of that general definition, and consultation with many specialists in the Bureau of Standards and other institutions, we developed a tentative priority list.

In May 1965 at Boulder, Colorado, under the chairmanship of Professor Condon, we convened a meeting of the Advisory Panel on Atomic and Molecular Properties. The panel looked at the tentative priority list we had, threw up its hands, tore it to pieces, and developed a new priority list which it then looked at more carefully and assigned some priorities. These priorities were based on three considerations: The importance of the topic to science and technology , or both; the need for additional compilers to do the job of evaluating and compiling the data in this particular area; and the availability in the published literature of data justifying an effort. There is no point in assembling a project if only a few scattered and irrelevant measurements are reported in the literature, even though the topic may be very important.

On this basis, the Panel developed a list of about 60 specific topics and assigned very high priorities to about 30.

I call your attention to a status report [1] which came out in 1968. You will find copies of this on the table in the Great Hall. This gives a more detailed description of some of the property categories and the projects as well which we have started in this program.

In the Status Report you will see the topics which we have been focusing our attention on.

Some of these areas were of immediate interest. We were able to identify in the National Bureau of Standards and in other places, data compilation projects with a substantial history of productivity. Then, of course, our concern was to relate these to additional topics which needed further consideration.

Very high priority was given to the topics of atomic energy levels and atomic spectral data. The Panel recommended that as far as fundamental constants went, the time was not ripe for additional

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(1) Status Report National Standard Reference Data System, April 1968, National Bureau of Standards, Technical Note 448, U. S. Government Printing Office, Washington, D. C. 70¢.

compilation or evaluation work. As you heard, this is going to be the subject of international activity in a year or two.

Another area of high importance was direct spectral data on atoms and molecules, specifically those areas of molecular spectroscopy which are very widely used in both research and industrial applications for the typical tasks of identifying materials and substances, process monitoring, etc. I am talking about infrared spectroscopy, ultraviolet, NMR, Raman, and mass spectroscopy.

The first advisory panel also identified some ongoing projects which were known to the specialists but not necessarily to some of us. The members suggested suitable participants for new projects which we might undertake and they gave us one very sound piece of advice; They recommended that, in several areas, we convene special ad hoc panels to seek further, more detailed advice from specialists on those topics.

This was intended to provide not only a closer look at what should be done, but how it might be done, and whether, in some cases, anything needed to be done. We found this device of the special ad hoc panel, focusing its attention on a particular scientific topic, to be invaluable.

We started a number of data compilation projects based on the Panel recommendation and on our communication with specialists in various fields. You can see, on display, some of the products which have come out since 1965. In the course of two years we learned enough so that we felt that another advisory panel meeting would be appropriate. In May 1967, Professor Condon again chaired an advisory panel which met here at the Academy and out at the National Bureau of Standards.

Because we had a better feeling for the broad scope of the program after three years of operation, we added some members to give more perspective. The property list was redefined and refined, and some of the priorities were changed. The panel listened to a summary of our problems and gave us specific instructions to place increasing emphasis, as our program developed, on high quality data.

This is not a surprising recommendation, but I would point out to you that one of our early concerns was to provide information wherever there was clear need for information. Because so much of atomic and molecular data is needed in areas of analytical and applied use, we had considerable difficulty in choosing between high quality data projects where there was not much data available and lower quality data where one can, in fact, sink in a morass of problems as to whether the information is worth presenting to the public even though it is all that is available.

We faced this problem from the beginning. I am sure any of you who are in data activities have to face it. Our concern has grown for the highest quality information and we now prefer to leave to other people responsibility for data of intermediate quality and applied utility.

In spite of limited funds, we now have data projects which cover a wide range of topics. Out of 34 currently assessed, high-priority topics, 20 are receiving attention from NSRDS-sponsored projects, and five additional high-priority topics are being covered under other sponsorship.

We have been fairly successful in getting products out. Our data compilers have completed and published 17 compilations of data and critical reviews, 12 bibliographies, usually carefully annotated and indexed, and one set of criteria for evaluation, which I will cover in more detail in a moment. There are at present six compilations in press.

This information now at hand in published form is emerging as an important intellectual resource. It is permitting us to evaluate the impact we can have in some special areas. In fact, we now see the opportunity, at least in some special areas, for our compilation projects to reach currency, and to get to the place where they are evaluating the literature as it comes out. This goal is not fully achieved in any area yet, but in some areas we see this on the near horizon, in the next few years.

This situation represents a substantial improvement because in most cases these projects started from scratch. We had one bibliography, for example, which covered 166 years, and when that was published in 1966 there was a big jump forward in currency.

Atomic transition probabilities are being covered in quite an up-to-date manner. Electron collision data, and molecular vibration frequencies are in fairly good shape, and X-ray emission wavelengths particularly are being evaluated on a fairly current basis.

In some other areas, it has been decided that there would be no data compilation program for a variety of reasons. For example, in mass spectrometry, we were advised that the instrumentation capabilities in this field were changing so rapidly that we should not at this time undertake any effort to evaluate and compile the information in the published literature. By the time the effort would be completed, our specialists told us, that information would be outdated by the more recent instruments now becoming available.

In the area of Raman spectroscopy, a similar point of view was taken because the advent of the laser light source has, in effect, outmoded much of the existing Raman spectral data.

In several areas, the National Standard Reference Program has focused national attention on the quality of data, and the efforts of our data project compilers to pull together the information have caused an upgrading in the quality of data generation.

I would like to mention one publication which brought about some very substantial interest in upgrading data generation.

One of our earliest projects was an attempt to collect existing infrared spectral data out of Government laboratories and other laboratories where there was no proprietary interest in the information, but for which there was no convenient distribution and publication channel.

In the course of that effort, which was operated by the ASTM, and a group of very competent spectroscopists, we found that we needed a clear-cut statement of evaluation procedures. We turned to the Coblentz Society and asked them to formulate rules for us. They developed and published [1] specifications for evaluation of infrared spectra which seem to be generally applicable.

They defined three categories of data: Class 1 data are those which are essentially physical constants of substances and are independent of the instrument on which the observations were taken. At the present time, there probably are no such infrared spectral data in existence over a range of wavelengths.

Class 2 spectra are the best which competent operators using current, modern instrumentation can produce.

Class 3 spectra are spectra which are useful for the identification of materials. For these spectra the substance must be well

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(1) Specifications for Evaluation of Infrared Reference Spectra by the Coblentz Society Board of Managers, Anal. Chem., Vol. 38, No. 9, August 1966, 27 A.

defined but more latitude is allowed in the instrumentation.

By indirection, Class 4 is everything else.

These concepts of Class 1, exceptional quality, Class 2 - as good as the current art can permit, and Class 3 something which is useful even if it is not perfect, have now become almost part of the language of data compilers in many different fields.

The interest in Class 2, as opposed to Class 3 infrared spectral data, has become quite substantial. In fact, professional spectroscopists, primarily in industrial laboratories, feel it a matter of pride to see if they can generate Class 2 data. They find it is not very easy, by the way.

In the area of nuclear magnetic resonance spectroscopy, it turned out that there was substantial interest in considerations of data quality. Our panel of evaluators and advisers, led by Dr. Barry Shapiro, suggested to us that the first thing was to find out what could be done and to develop some inter-laboratory comparisons. That program is now going on.

Other accomplishments to date include the substantial cooperation from scientific and professional societies of a wide variety, major ones like the American Chemical Society, small special ones like the Society for Applied Spectroscopy, and so on.

We have now developed the basis for a national cooperative effort. We are very far from achieving full cooperation, but many segments of the country know about and try to become a part of this effort.

As I mentioned before, we have found that special panels give us a major advantage in that they provide a low-cost, low-key effort beginning consideration of a field. There is one problem, and that is that the effort won't stay low-key and low-cost. You get a group of enthusiasts together and they develop a program for you. Then they come back and say, "Well, okay, we told you what to do; now how about some funds so we can do it." In a time of restricted funds it is hard to say no to them, but it is even harder to say yes.

Subject to funding limitations, we see that it is going to be possible to develop an adequate program and that our current way of doing this, turning to specialists, starting small projects, watching them grow, seems to be adequate for this development.

The features of the future program will be continuing primary emphasis on selected data compilations and critical reviews, and expanded effort to define and publish criteria for data compilation and generation; exploration of the utility of high quality data; how much does it mean to the large majority of data users to have better data as opposed to the data they have been used to getting?

How much do they want their data generation effort to be improved? Are they willing to look at higher quality data then they, themselves, generate? What does it mean to strain the limits of current instrumentation? Will it be necessary to involve computers with these various instruments which obtain most of this data?

Other plans for future action are based on our recognition of a need for better publicity for our products. Time after time I find that the data compilers and data specialists may know about our output, but the users don't. We see a need for displays of our products and descriptions of our activities at technical meetings. We see a need to involve the services of commercial publishers, because they are far more capable than a Government program is to publish and promote, advertise and generally sell the products which we consider to be of value.

We see the need for a two-way communication with individual users, feedback from them as to whether we are satisfying their needs. We understand the need to relate to specialized information centers and retailers of information, such as those being developed by other Government programs. I am speaking specifically of the National Science Foundation now, which is setting up at the University of Pittsburgh a Chemistry Information Center and one on physics at Stanford University. We feel it may be important to relate to industrial information divisions, in-house information services, as ways to reach our individual users. Many industries have such activities, and we would like to tie in with them to become a source of prepackaged information for them to utilize.

It is difficult, however, to do this on a systematic basis, because the development of this communication takes time. Many of these information groups feel that they may, perhaps, suffer in their proprietary fields of interest if they set up too close a two-way communication.

I invite your participation in our effort to try to talk to the industrial information activities, to set up meaningful programs of the kind they want. We have no preconceived notions as to what we should give these people. We are willing to play the tune the way they want it played, but do have to know about them; we have to communicate in some way.

Finally, there is a real need for us to study the value of the capability to answer questions from outside on the spot, to get a letter and to either answer it ourselves or refer it to an information analysis center for prompt answering. Is that more effective than publication of information?

These are some of the questions which you, in your communications with us, can help answer.

Thank you.

DR. SCHULMAN: Now that this year has brought into focus the establishment of the office by legislative action, do you see in the coming years, starting with this year, any change in your operation, any change in priorities and emphasis?

DR. ROSSMASSLER: Yes, I see one in particular and that is that the legislation gives us a chance to try to answer on a tentative basis one of these questions I asked just now, namely, the problem of involving publishers who can provide additional methods of disseminating our products. We can see the probability of a change in our marketing procedures, but no significant change, I think, in our internal priorities program.

DR. SCHULMAN: Do you see a quickening of the pace in such a huge and complex program?

DR. ROSSMASSLER: We hope to see a quickening in the pace. In the present economic environment, we can't make any predictions.

DR. BRADY: If there are no further questions, we will proceed to the next topic. Perhaps as we go along some other questions will occur. Don't hesitate to ask questions or to make comments on any subject following any talk.

The second area of maximum emphasis for our program has been that of thermodynamics and transport properties. These will be covered by Dr. Howard J. White. He will also discuss the area of surface and colloid properties, which is one of our lower priority areas, but is also his responsibility. Dr. White?

THERMODYNAMIC AND TRANSPORT PROPERTIES; COLLOID AND SURFACE PROPERTIES

By

Dr. Howard J. White, Jr.

DR. WHITE: As Dr. Brady has pointed out, I am wearing two hats. One is considerably larger than the other. I will cover both programs with perhaps 85 percent of the emphasis being on thermodynamics and transport properties.

Thermodynamics and transport properties, since it received the second highest priority among the various areas considered in the initial setting up of the NSRDS, has received considerable financial emphasis also.

In 1964, and again in 1965, panel meetings were held here at the Academy. In these meetings the priorities of study and, more importantly in the case of thermodynamics, the names of people who were already involved and interested in this area were brought to light. I think a moment's reflection will show that thermodynamics, by its very nature, doesn't require as much priority setting, as perhaps atomic and molecular properties because it all fits together into one whole, so to speak.

One set of priorities that was definitely established was that major emphasis should be given to the heats and entropies and free energies of formation of substances in their standard states and in other states as well, and this has been done. Such data are necessary in considering chemical equilibria.

The whole program has been modulated by the existence of previously established programs and the availability of funds, which is a very good modulator.

Colloid and surface properties have a lower priority. We were fortunate, in the case of colloid and surface properties, that the National Academy had a Committee on Colloid and Surface Chemistry which had already, of its own initiative, planned a program of data evaluation in the field, so that we were able very early to assist this ongoing program. This NRC committee that functioned to establish this program now serves as one of our advisory panels. Actually, the very first projects that we got were projects that were already going on on a voluntary basis.

(Slide 1)

THERMODYNAMIC AND TRANSPORT PROPERTIES

Technical Areas

1. Heats, Entropies, Free Energies of Formation, Heats of Transitions, Specific Heats, and Related Physical Properties

2. Gases, PVT, Critical Region

3. Liquid Non-Electrolytes, Liquid-Vapor Equilibrium

4. Liquid Electrolytes, Fused and in Solution

5. Solids, Solid-Liquid Equilibrium

6. Transport Properties

In this first slide I have divided thermodynamics and transport properties up into the six somewhat arbitrary categories.

Number 1 is listed because it was specifically established as a high-priority area. The others include most other areas of the field of current interest.

(Slide 2)

THERMODYNAMIC AND TRANSPORT PROPERTIES

Programs by Technical Area

1. Heats, Entropies, Free Energies of Formation, etc.

Thermochemical data inorganic compounds including IUPAC Bulletin of Thermodynamics and Thermochemistry

NBS	Wagman

Thermochemical data organic compounds including IUPAC Bulletin of Thermodynamics and Thermochemistry

Texas A&M	Zwolinski

Low temperature heat capacities

NBS	Furukawa

In the second slide the program in the first technical area is presented. The IUPAC Bulletin of Thermodynamics and Thermochemistry was included because this is, in fact, an important effort of two of our major centers. It is, I am sure, an effort that a good number of you are aware of, although perhaps not aware of the participation of the Office of Standard Reference Data in its production and sponsorship.

The two groups at the top of the list are large data centers that existed before the establishment of the NSRDS, as Dr. Rossini pointed out earlier. The last one is a smaller activity, more specifically concentrated on heat capacities.

(Slide 3)

THERMODYNAMIC AND TRANSPORT PROPERTIES

Programs by Technical Area

2. Gases, PVT, Critical Region

Thermodynamic properties of polar gases (ammonia)

NBS	Haar

Thermodynamic properties of organic compounds

Texas A&M	Zwolinski

3. Liquid Non-Electrolytes, Liquid-Vapor Equilibrium

Vapor-liquid equilibrium (less than 2 atms)

U. of Detroit	Canjar

Vapor-liquid equilibrium (more than 2 atms)

Cal Tech	Sage

The program in the second technical area is shown on the next slide. Mr. Harr at NBS has a general assignment on thermodynamic properties of polar gases and is currently working on ammonia; presumably as time progresses, he will go on to other polar gases.

I have mentioned Dr. Zwolinski's efforts again here. I could also have put him in the next category.

The next technical area is covered in Slide 4.

(Slide 4)

THERMODYNAMIC AND TRANSPORT PROPERTIES

Programs by Technical Area

4. Liquid Electrolytes, Fused and in Solution

Fused salt properties; conductance, density, viscosity, electrochemical cells, surface tension

RPI	Janz

Aqueous and non-aqueous solutions

NBS	Hamer

5. Solids, Solid-Liquid Equilibrium

High temperature properties and decomposition of inorganic salts (carbonates)

NBS	Stern

High temperature metal-metal oxide systems

MIT	Elliott

High pressure data center

Brigham Young	Hall

Phase diagrams of binary alloys

IITRI	Parikh

The first item is a program at Rensselaer Polytechnic Institute. There has been quite a bit of activity in this area at RPI. We have a product about to come out on the conductivity, density and viscosity of some 100-odd fused salts. There has also been some work on the EMF's and hence the free energies of formation, and also some work on surface tension.

As we go to the solid state area, one should bear in mind that we have a technical area named "Solid State," so some programs that might occur to you as logical inclusions here are not present and the same will be true of transport properties, because of the arbitrary division that we effected between the two areas where there was a substantial overlap.

(Slide 5)

THERMODYNAMIC AND TRANSPORT PROPERTIES

Programs by Technical Area

6. Transport Properties

Transport properties of fluids

NBS	Hanley

Thermal conductivity

TPRC-Purdue	Touloukian

Viscosity and thermal conductivity of liquids and gases

Northwestern	Thodos

The next slide shows our program in transport properties. We have a program on the transport properties of fluids, which is primarily concerned with moderately dilute gases, covering all transport properties, correlating through various kinds of intermolecular potentials. We have thermal conductivity compilation work at the Thermophysical Properties Research Center in Purdue, under Dr. Touloukian.

Thermal conductivity and viscosity of gases and liquids is a small program that has just been initiated fairly recently under Dr. Thodos at Northwestern.

These programs are all still in existence and they cover almost all of the programs that have been started in thermodynamics and transport properties. This is partly the result of the nature of the program, by which I mean that you can't get things done in a great hurry, and partly from the guideline that we were given emphasizing the importance of continuity in this type of operation.

(Slide 6)

COLLOID AND SURFACE PROPERTIES

1. Solid-Liquid and Solid-Gas Interfaces

Electrical properties of interfaces

Agricultural University, Wageningen, The Netherlands — Lyklema

Data pertaining to phase-transition kinetics

Stanford — Pound, Tiller

2. Liquid-Liquid and Liquid-Gas Interfaces

Surface tension of liquids at ordinary temperatures

Wayne State — Jasper

Surface tension of liquid metals

RPI — Janz

3. Dispersions of Colloidal Particles

Light scattering of liquids

Clarkson — Kratohvil

Critical micelle concentrations

Wisconsin — Mysels, Mukerjee

Slide 6 shows the entire program in colloid and surface properties. All of the projects that are mentioned here are part of the program of voluntary projects started by the Committee on Colloid and Surface Chemistry of the National Academy of Sciences which have been given funding to enable them to move faster, with the one exception of the project on data pertaining to phase transition kinetics under Professors Pound and Tiller at Stanford University. All of the rest of them were either in existence at the time the NSRDS program was started, or were waiting funding at that time.

In the next slide I have listed our finished products. We have nine published monographs of various types. There are five in press. We have four that are in the final revision stages, two that have been published in a different area but are of specific interest in one of these two areas, and then there is another category that could have been listed here, namely, two continuing programs to make data available - - the IUPAC bulletin I mentioned earlier, and the successor to the MCA program which is now called the TRC Data Program. We provide substantial support to these two activities which do not come out as NSRDS reports, per se.

(Slide 7)

PUBLICATIONS

THERMODYNAMIC AND TRANSPORT PROPERTIES

COLLOID AND SURFACE PROPERTIES

Published	9
In Press	5
Final Reports in Review or Revision	4
Published in Other Areas But of Interest in One of the Above Areas	2

A full listing in the first two categories will be made available.

Now, as far as the future is concerned, I suffer somewhat from following Steve Rossmassler in that the needs and ideas and thoughts he mentioned are not exclusive to any particular discipline.

We are serving more and more as a focal point for data activities within the United States, and more recently, with the onset of some international activities, we are beginning to get some coordination and cooperation with some specific projects in other countries -- I am thinking particularly of the program under Dr. Angus on industrially important gases, with which we intend to cooperate insofar as we can.

As additional funds become available, we expect additional growth. I think it will probably be modest for the immediate future, but we have hopes nonetheless.

The development of criteria, which was mentioned several times, has happened more or less spontaneously in this program. There is no product out of the nature of the Coblentz Society's publication; however, there was a meeting about a year ago on the evaluation and presentation of experimental data on thermal conductivity in fluids, and I think that some product from that group will appear in the immediate future.

Thank you.

DR. BRADY: Are there questions or comments?

DR. SCHULMAN: Is Beckman of the University of Maryland collaborating with you in the transport properties program?

DR. WHITE: In an indirect way. He was part of the NASA program that we were working closely with.

DR. BRADY: Funded by the man who asked the question'

DR. SCHULMAN: All I am saying is that the program was recommended to us by your office and I would hope that it is not being neglected.

DR. WHITE: No - it is not being neglected.

DR. BRADY: We have our problems, Fred, dispersing our resources in many different places!

One of the reasons the nuclear property category has not been emphasized by our program is because the Atomic Energy Commission, throughout its whole history, has been active in promoting data compilations of various kinds. The Chairman of our Nuclear Advisory Panel, which met a week or two ago here at the Academy, made the comment that it is often said that in the nuclear field the data compilation situation is in better shape than in most of the other fields of science. If this is true, he says, God help the other fields.

Dr. David Goldman is the program manager for nuclear properties in the Office of Standard Reference Data. He is also a member of the Reactor Division at the National Bureau of Standards, working only a minor fraction of his time in the Office of Standard Reference Data. He is a well known data compiler himself, and is responsible for the General Electric chart of the nuclides, including the most recent addition, which is about to appear since he joined the National Bureau of Standards. Dr. David Goldman.

NUCLEAR PROPERTIES

By

Dr. David L. Goldman

DR. GOLDMAN: As Dr. Brady pointed out in his introduction, the field of data compilation for nuclear properties is really better covered than most due to the presence of one all-encompassing agency which has direct responsibility for the compilation, evaluation, and dissemination of nuclear data. This governmental organization is, of course, the Atomic Energy Commission, Thus, our office at the National Bureau of Standards has not provided directly for the funding of any particular nuclear data operation, with the exception of one center established at the National Bureau of Standards. The Photonuclear Data Center under the directorship of Dr. Everett Fuller. This data center has published two annotated bibliographies of references to journal articles containing photonuclear data.

In addition, the Office of Standard Reference Data has provided liaison, advice, and assistance to the Atomic Energy Commission primarily in assisting individuals in the AEC in planning their programs, in evaluating the programs, and in providing suggestions where additional support ought to be given, and to what extent. We have performed this assistance in conjunction with the Office of Critical Tables, arranging for panel meetings composed of experts who generate or use nuclear data.

The panels have met three times in the past 3-1/2 years, the most recent meeting a week and a half ago in the other building, the Joseph Henry Building, of the National Academy of Sciences.

To give you an idea of how these panels meetings work, let me briefly just summarize the kinds of recommendations which were sought at this recent panel meeting and just briefly what the recommendations of the panel meeting will be, or at least presumably will be, when they are committed to a final report.

The Atomic Energy Commission has been providing a fair amount of money through the years for the compilation and publication of nuclear data, especially for the radioactive properties and energy levels of nuclei. This work has been carried out by the Nuclear Data Group which was headed by Dr. Kay Way of Oak Ridge National Laboratory her recent retirement. Dr. Way is still quite interested in this field and continues as editor of the journal Nuclear Data which publishes selected compilations and evaluations of nuclear data.

This large, ongoing effort of the Nuclear Data Group is published as the "Nuclear Data Sheets", presently Section B of "Nuclear Data". There is, in addition, the well known effort initiated by the present Chairman of the Atomic Energy Commission 20 years ago to compile and evaluate the radioactive properties of nuclei. The sixth edition of the Table of Isotopes which appeared in 1967 is a book of six hundred pages, which nevertheless could be published as a part-time undertaking of two or three nuclear chemists. However, the realization that a continuation of this particular project would necessitate the computerization of the data files, and the automation of the publication procedure, and, therefore, required direct funding from the Atomic Energy Commission.

One of the subjects that we presented to the panel was whether duplication existed between these two activities receiving support from the Atomic Energy Commission and whether such duplication was sufficiently great that perhaps only one effort should be supported. The conclusion was that at present the two different groups served different kinds of scientific and technological publics and, therefore, both efforts ought to be supported with the proper amount of laision and cooperation between the two so as to avoid such duplication of activities involved in such things as preliminary scanning of the literature and perhaps even preliminary evaluation of the data.

In addition, the panel was apprised of the status of a variety of other large and major supported efforts such as the recently established Brookhaven National Neutron Cross-Section Center, which compiles and evaluates neutron cross-sections and publishes this primarily as data tapes for use directly in computers.

Progress relating to the CINDA Annotated Bibliography on Neutron Cross-Section Data was also discussed at the panel meeting.

In addition to providing assistance or advice to the Atomic Energy Commission, the Office of Standard Reference Data cooperates with other agencies both in the United States and abroad in presenting the overall picture in the field of nuclear data, specifically, the Defense Atomic Support Agency of the Department of Defense, and the two major international organizations, the European Nuclear Energy Agency and the International Atomic Energy Agency.

This cooperation is maintained by joint publication, joint communications, and meetings. Recently the Office itself has undertaken the publication of two compilations, one in the compilation and evaluation of thermal neutron cross-section data for all isotopes which have been measured, and a revised table of the properties of nuclei.

Last, and certainly not the least, we attempt to make available the general services of the Office to various individuals or groups who might benefit by them. I have in mind specifically the expertise available in this office in terms of automatic data storage, and especially automated printing procedures which have been developed by another member of this Office, Joe Hilsenrath. He will be talking in much greater detail, I am sure, about these specific activities.

It is hoped that in the future, with the acquisition of more money, this particular program will be able to supply more than just our best wishes and advice, but indeed some funding to the various compilation and evaluation groups to assist them in properly carrying out their missions.

DR. BRADY: We have a question at the back of the room?

QUESTION: If someone needs data on cross-sections, is your office the place to write to get the latest information on available compilations?

DR. GOLDMAN: For that specific kind of data, the answer is yes. It turns out that people frequently do write to the office for specific information. We do not at present have everything available for immediate dissemination, but I think I can say without exception that people can be referred to the specific center which might make this information available. For the question you may have, either our office could supply the answer, or, the Brookhaven Neutron Processing Center.

DR. BRADY: Thank you, Dave.

The next two categories of properties to be discussed, solid state properties and the properties of chemically reacting systems, are under the program managership of Dr. Lewis H. Gevantman, who has been with the office approximately a year and a half, now, and is a physical chemist by background.

Dr. Gevantman.

SOLID STATE AND CHEMICAL KINETICS

by

Dr. Lewis H. Gevantman

DR. GEVANTMAN: This afternoon, I think it useful to break up the discussion into a short review of the history of each program area, what has been achieved to date, and follow this up with a word or two on where we are going.

I think that before launching into the two areas named by Dr. Brady, I would mention briefly the last program area that was on the slide that Dr. Brady showed you and tell you that we do intend to start a program in the area of mechanical properties. To date, we have not gone beyond the listing of the properties that we would examine were we to initiate work in that area.

I was delighted to hear about the activity in this field from Dr. Speight and Dr. Lyman and hope that we can keep in touch with their activities, until we initiate some of our own.

To give you some idea of our thinking in this area, I have listed the materials and their properties below. "Mechanical Properties List" (see Annex II, pages 148-151)

Now let's go on to discuss two additional program areas that are on the program. The first is Chemical Kinetics. This activity was initiated several years ago when an NAS-NRC Advisory Committee under the chairmanship of Dean Henry Eyring was called on January 17, 1964. The committee was charged with the responsibility of advising the Office of Standard Reference Data on which programs could be undertaken in the field of chemical kinetics to produce the type of information which would most benefit the community. In making its recommendations, the committee endorsed a memo which was prepared for the committee's consideration. (Refer to AnnexIII, pp. 152-156)

The Commiteee met again on an ad hoc basis on March 30, 1966, under the Chairmanship of Dr. M. B. Wallenstein and reiterated the views expressed in the earlier meeting. I should like to show very quickly the type of programs that the Committee recommended so that you may see for yourselves the wide range of subjects covered. (Slides 1, 2 and 3)

In addition to outlining the program areas, and the monographs that should be produced the committee recognized the value of establishing data centers which could review the published literature and supply information upon request to those people who would write critical monographs, thereby making the task of the evaluator less time consuming in reaching his desired goal. With that in mind, the office encouraged the formation of data centers in the kinetics area. One is located at the National Bureau of Standards in Gaithersburg, under the direction of Dr. David Garvin. The other is the Radiation Chemistry Data Center under direction of Professor Milton Burton, Head, of the Radiation Laboratory at the University of Notre Dame.

Very briefly, the aim of the Chemical Kinetics Information Center was to develop a storage and retrieval system for the collection of papers and reports related to rates of chemical reactions, photochemistry, and inelastic scattering. The input of such information involved the selection, evaluation, indexing and storage of the pertinent material. This activity, initiated a number of years ago, has gone from manual operation to the present system which involves the use of the computer for the storage and retrieval of the information. The center's activities include then, the storage of chemical kinetic data, responding to inquiries on kinetic data, making the kinetics community aware

PROGRAM FOR CHEMICAL KINETICS

I. Homogeneous Reactions

A. Gas Phase

1. Elementary reactions

a) Elementary steps with stable molecules
   i) Unimolecular reactions
   ii) Bimolecular reactions
b) Energetic species production
c) Atom reactions in simple radicals
d) Atom - radical reactions
e) Molecule - ion reactions
f) Free radical steps

2. Relaxation processes

a) Vibrational relaxation
b) Rotational relaxation

3. Quenching of fluorescence

4. Photo-chemical primary processes

5. Vacuum UV photo chemistry

6. Radiation chemistry

7. Electric discharge reactions

8. Fast reactor kinetics

*9. Cross-sections for atomic collisions

a) Heavy-particle/heavy particle interactions
b) Processes involving
   i) Electric and magnetic field excitation
   ii) Dissociation
   iii) Ionization
   iv) Detachment

* This topic could be assigned to either the Atomic and Molecular Properties Area or the Chemical Kinetics Area. Since the operational approach being considered has more in common with other projects in the former area than in the latter, it is listed here for cross-reference purposes only.

B. Liquid Phase

1. Acid-base catalysis

2. Oxidation - reduction reactions
   a) Metals
   b) Non-metals

3. Electron transfer

4. Proton transfer

5. Radiation chemistry
   a) Aqueous
   b) Organic
   c) Isotope reactions

6. Organic reactions
   a) Carbonium steps
   b) Carbonium ion steps
   c) Sulfonation
   d) Hydration
   e) Hydrolysis
   f) Peroxide reactions
   g) Kinetics enzyme

7. Substitution reactions of coordinate compounds
   a) Labile centers
   b) Non-metal centers
   c) Metal centers
      i) Coordination number 6-8
      ii) Coordination number 4

C. Solid Phase

1. Solid state diffusion

2. Photo reactions

*3. Particle penetration thru matter

* This topic could be assigned to either the Atomic and Molecular Properties Area or the Chemical Kinetics Area. Since the operational approach being considered has more in common with other projects in the former area than in the latter, it is listed here for cross-reference purposes only.

II. Heterogeneous Reactions

A. Gas-Liquid

B. Gas-Solid

1. Reaction of steam and other gases with metal surfaces: 1000° - 2000°K

*2. Adsorption - desorption phenomena

*3. Reactions at surfaces - catalysis

C. Liquid-Solid

1. Electron transfer at electrodes

*2. Reactions at surfaces - catalysis

*These topics are within the scope of the program of the Colloid and Surface Properties Area, and are listed here for cross reference purposes only.

of data publications in the field and coordinating its activities and knowledge with those of other data centers in the chemical kinetics field. Similarly, the Radiation Chemistry Data Center has aimed toward developing a similar capability in radiation chemistry. This activity is not quite as far along in its development as is that of the data center at NBS. The next slide will show you how the center functions. (Slide 4) The input information is recorded on paper tape then on to magnetic tape, from which bibliographies are produced. A weekly list of papers in radiation chemistry is produced and issued every week. Literature searches are conducted and, of course, the data that is taken from the papers is put on cards and filed for future reference. The intent is to incorporate these data into an automated storage and retrieval system.

This then, gives you a very brief description of what we now have. Let us examine the output and progress to date. The Office of Standard Reference Data has sponsored the publication of a number of monographs in the field of chemical kinetics. To date, it has published three which are among the publications displayed in the lobby. They are:

NSRDS-NBS-13 - "Hydrogenation of Ethylene on Metallic Catalysts" by J. Horiuti

NSRDS-NBS-9 - "Bimolecular Gas Phase Reactions" by A. F. Trotman-Dickenson

NSRDS-NBS-20 - "Gas Phase Reaction Kinetics of Neutral Oxygen Species" by H. S. Johnston

In addition, we have three manuscripts that are in varying stages of completion and we expect them to be issued shortly. They are:

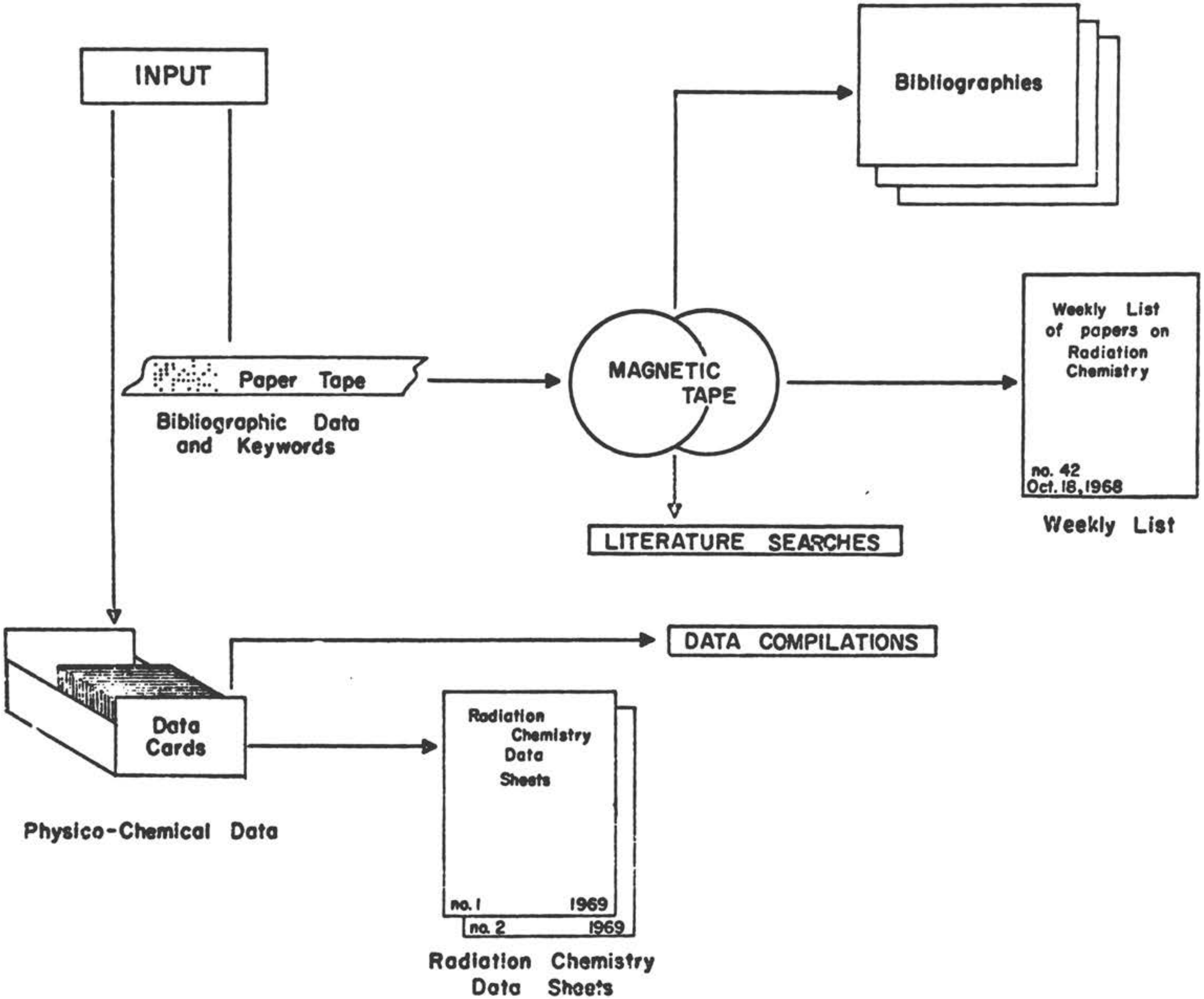
"Bond Dissociation Energies for Simple Molecules" by R. de B. Darwent

"Critical Review of Rate Constants of Reactions in Re-Entry Flow Fields" by M. Bortner

"Kinetic Data on Gas Phase Unimolecular Reactions" by S. W. Benson and H. F. O'Neal

Additionally, contracts for manuscripts have just recently been negotiated that will be published within the next few years. In addition, I would point out to you a number of publications which have been put out

RADIATION CHEMISTRY DATA CENTER



in the other program areas which relate closely to the field of chemical kinetics. To read just a few, they are:

W. F. Wilson - "Hydroxyl Radical Reactions in the Gas Phase"
L. F. Dorfman - "Review in Hydroxyl Radical Kinetics in Water"
J. T. Herron - "Rate Constants for O Atom Reaction with Organic Compounds"

A. Publications Issued in the NSRDS Series:

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

Tables of Molecular Vibrational Frequencies, Part 1, by T. Shimanouchi, NSRDS-NBS-11 (40 cents)

Tables of Molecular Vibrational Frequencies, Part 2, by T. Shimanouchi, NSRDS-NBS-11 (30 cents)

Tables of Molecular Vibrational Frequencies, Part 3, by T. Shimanouchi, NSRDS-NBS-17

Critical Evaluation of Ion Appearance Potentials, Ionization Potential and Ion Heats of Formation, by J. L. Franklin, F. H. Field, J. Dillard, H. M. Rosenstock, and F. N. Harllee.

B. Other NBS Compilations of Data

Electron Impact Ionization Cross-Section Data For Atoms, Atomic Ions, and Diatomic Molecules: 1. Experimental Data, by L. J. Kieffer and G. H. Dunn, Published in "Reviews of Modern Physics 38", No. 1-35 (Jan. 1966). Also to be bound with related material in the NSRDS Series.

Critical Review of Cross-Sections for Electron Excitation of Atoms by Electron Impact, by B. Moiseiwitch (to be published in "Reviews of Modern Physics", Jan. 1968).

Electron Impact Ionization Cross-Section Data for Atoms, Atomic Ions, and Diatomic Molecules: II, Theory and Comparison of Theory and Experiment, by M. Rudge, L. J. Kieffer, and G. H. Dunn (to be published in "Reviews of Modern Physics" Jan. 1968).

Compendium of Ab-initio Calculations of Molecular Energies and Properties, by M. Krauss.

C. Nondata Publications from NSRDS Related Projects:

Bibliography of Low Energy Electron Collision Cross-Section Data, by L. J. Kieffer, NBS Misc. Publ. 289 (50 cents)

Bibliography of Atomic and Molecular Processes for 1963, by C. F. Barnett, J. A. Ray, J. C. Thompson, and F. W. McDaniel, ORML-AMPIC-1 (July 1965)

Bibliography of Flame Spectroscopy, Analytical Applications, 1800 to 1966, by R. Mavrodineanu, NBS Misc. Publ. 281 ($2)

A Bibliography on Ion-Molecule Reactions, Jan. 1966 to March 1966, by F. N. Harllee, H. M. Rosenstock, and J. T. Herron, NBS Tech. Note 291 (30 cents)

In addition to the activities of our office, I should also like to mention that the data centers have also been active in publishing data. Over the years, the Chemical Kinetics Information Center has issued a number of important publications some 50-60 I believe and there has been a very important compilation of evaluated and estimated rate coefficients published by Dr. Garvin in which about 1500 reactions are listed. The center has also transferred the IDA Bibliography on, "Atom and Light Molecule Cross Sections" into the NBS collection. This represents some 5, 000 bibliographic entries.

Dr. Garvin, himself, is very active in the evaluation, and in the coordination of his activities with other groups. He has written a paper on how to evaluate chemical kinetic rate constants and serves as a consultant on the preparation of critical monographs in this field. The Radiation Chemistry Center has built its activities from the simple indexing of papers to the activities which I have shown you on the slide. To date, they handle some 2500 items per year. They have also converted approximately 1800 of these to magnetic tape and have stored radiation chemical information originally contained in the Dow Chemical Company compilation into their system. (18000) They have also prepared and issued a large number of bibliographies (15-20) in the field of Radiation Chemistry at the request of people in the field and are stimulating the preparation of data sheets to cover reactions of those molecules whose decomposition mechanism is better understood.

Dr. Burton is also editing a series of papers covering a wide variety of subjects in the field of Radiation Chemistry.

In addition to the activities listed above the data centers are also trying to coordinate their activities with one data center outside the U. S. I refer to the High Temperature Reaction Rate Data Center in the Department of Physical Chemistry at the University of Leeds. This data center is supported by the Office of Scientific and Technical Information and is under the direction of Dr. D. L. Baulch. This group has issued its first report which reviews and evaluates eight reactions of carbon monoxide and carbon dioxide with a number of atoms and radicals. The centers are also in close touch with the Chemical Kinetics Working Group of the Interagency Chemical Rocket Propulsion Group. This group is also attempting to compile rate data of particular interest to propulsion research.

Finally, I would mention the group at the Joint Institute for Laboratory Astrophysics which compiles and evaluates information in the field of Low Energy Atomic Collision Cross Sections. The work that they do impinges on the work of the Chemical Kinetics Center. Of course one may say the same about the activities in Atomic and Molecular Properties and in Thermodynamics as well.

This then, brings me to the future. I have already indicated that the critical monographs work is proceeding and we are on the constant lookout for experts to author articles of interest in the field. At the present time, we are negotiating with a number of other individuals for future preparation of reviews covering oxygen nitrogen reactions in the atmosphere, the kinetics of unimolecular reactions in the non-equilibrium region, the examination of theoretical and experimental techniques used in the evaluation of rate constants and so on. We are also interested in the establishment of a data center on solution kinetics. We plan additional ad hoc advisory committee meetings to cover small program areas in the field of kinetics. For example, I believe the time may be ripe to examine the photochemistry area. We also seek an enlargement of our international relations through the use of bilateral exchanges a subject which has already been covered by Dr. Brady. This then, is what I have to tell you to date about our chemical kinetics program. Because of the shortness of time, I should like to go on then to the next program area - that is the Solid State Properties Program.

SOLID STATE PROPERTIES

The origin of this program is similar to the chemical kinetics program. That is, an NAS-NRC Advisory Committee was established, and convened on February 8, 1965. The committee was charged with the objectives contained on the next slide (Slide 5)

The deliberations and final recommendations of the committee was the production of a list of properties which could be compiled in the field of solid state. Additionally, the committee assigned priorities on the basis of importance, lack of existing data and the timeliness or ripeness of compiling such data. The next three slides show the criteria employed and the property list recommended by the committee. (Slides 6, 7 and 8)

Over the years, a number of projects have been undertaken to conform to the recommendations outlined by the committee. The type of activities again include the production of evaluated data as well as the establishment of data centers to deal with the wide variety of subject matter indicated in the slides. To mention a few, there is a data center and evaluation presently underway in the single crystal data area. The intent is to update and issue a 3rd edition of the book by Professor J. D. H. Donnay. This book will be issued in two volumes and will contain some 30,000 entries. The center is compiling the information using the combined efforts of a number of people both nationally and internationally. Another aim of this project is to print the book by computer. The center's activities are under the direction of Dr. S. Block and Dr. H. Ondik.

A number of other data centers have also been established principally at the NBS. The Alloy Data Center is under the direction of Dr. L. H. Bennett and Dr. G. C. Carter, In addition to the compilation of data, Dr. Bennett is in the process of evaluating Knight-shift data with the aim of producing a critical monograph in this field. This will be published in the 1968 Magnetism and Magnetic Materials Digest - published by Academic Press.

Another activity in the critical monograph area is the evaluation of soft x-ray spectroscopic data by Dr. J. R. Cuthill. Another data center is the Cryogenics Data Center at Boulder under the direction of Mr. V. Johnson, which is compiling some of the properties of extremely pure metals. Another data center is compiling information in the diffusion of metals and alloys. This data center is under the direction of Dr. J. R. Manning.

Finally, there is a data center which compiles information on the properties of superconductive materials. This project is under the direction of Dr. B. W. Roberts at the General Electric Company.

RECOMMENDED OBJECTIVES FOR

SOLID STATE PANEL DELIBERATIONS

1. A list of those properties which are considered in the domain of solid state physics.

2. A list of those properties in 1. (above) which are amenable to compilation, i.e. which of the properties in 1. are the available data of sufficient precision to warrant compilation and critical evaluation.

3. List of existing compilations and identification of groups currently engaged in compilation activities on properties in 1.

4. Develop a schedule of priorities of data compilation of those properties listed in 2. (above) which are considered most needed by the scientific community, industry or technology.

5. Recommendations or suggestions of competent individuals or groups who may be interested in data compilation.

Criteria for Priority Assigned
by
Solid State Advisory Committee

1st digit: importance (scientifically & technologically)

high	A
medium	B
low	C

2nd digit: lack of existing

high	A
medium	B
low	C

3rd digit: ripeness

high	A
medium	B
low	C

Monograph - M

Property List	Priority
Thermal:	
Density	AAB
Diffusion Coefficient	ACA
Heats of Transition	AAA
Lattice Energies	ABA
Distribution Coefficients	ABA
Cohesive Energies	ABA
Debye Temperatures	AAA
Gruneison Constants	AAA
Electronic Specific Heat	AAA
Heats of Transition	AAA
Surfaces:	
Work Function	ABA
Contact Potentials	ABA
Surface Energies	AAA-M
Structural:	
Crystal Structure	ACA
Symmetry Elements	AAB
Ionic Radii	ACA
Interatomic Distances	ACA
Dislocation Parameters	ACB
Defect Parameters	ABB-M

Property List	Priority
Optical:	
Soft x-ray Spectra	BBB
Spectroscopy of Solids	AAA
Infrared Spectra	AAA
Electronic Energy Gap	ABA
Refractive Indices	ABA
Fermi Surfaces	BBB-M
Electrical:	
Ionic Conductivity	AAB
Hall Coefficients	ABA
Thermoelectric Coefficient	BAA-M
Resistivity	AAA
Magneto Resistivity	BBA
Photoelectro Magnetic	BCB
Dember Potential	BCC
Superconductivity	ABB
Dielectric Constant	AAB
Polarizability	AAC
Ferroelectrics	BBC
Carrier Lifetimes	AAC
Magnetic:	
Spin Lattice Relaxation	ABA
Saturation Moment	AAA
Anistropy	AAA
Magneto Striction	AAA
Magnetic Transitions	AAA
Transition Temperature	AAA
Magnetic Structures	AAA
Magnetic Susceptibilities	ABA
Gyromagnetic Ratio	AAA
Internal Fields	AAA
Mechanical:	
Elastic Constants	ABA
Reststrahlen Frequency	AAB
Phonon Spectra	AAA
Velocity of Sound	AAB
Shear Modulus	ABB
Bulk Modulus	ABB

Let us now proceed to examine what has been produced to date. We have in print a publication by Dr. Roberts on the superconductive properties of a number of material compounds (Tech. Note 408), the Resistivity of 16 pure metals in the temperature range 0 to 273 °K by L. A. Hall (Tech. Note 365), and a description of the Alloy Data Center (Tech. Note 464). A number of manuscripts are being processed for publication.

At the present time, we have another version updating of the superconductive properties of materials by Roberts. We have information on the Knight Shift and Soft X-ray Spectroscopy being compiled. We will soon issue the book on Crystal Data. Another work soon to be published is Thermal Conductivity of Materials at Low Temperature by R. L. Powell. Under our P. L. 480 program using counterpart funds in India, we have two projects, one under the direction of Dr. S. C. Jain who is compiling tables of Defect Properties of Non-Metallic Crystals and Dr. C. N. R. Rao who is compiling a bibliography of Phase Transformations in Solids.

In the future we hope to initiate additional data centers covering some of the properties outlined. For example, we are asking Professor Friauf of the University of Kansas to prepare a monograph evaluating data on diffusion and ionic activity in crystals and halides. The review will collect data on these two phenomena and indicate those properties of defects which are responsible for these phenomena.

We have also, from time to time, considered such simple activities as the issuance of a data sheet on the properties of a single element. And of course we continue to search for experts willing to compile and evaluate data in those areas where such activities will produce useful results. We solicit those of you in the audience who are interested in doing so to contact us so that we may examine the possibility of such efforts. This then, is a very brief and hurried description of the activities in three of our program areas. If there are any questions, I shall do my best to answer them.

QUESTION; Is the Donnay crystal data project now attached to your office? It has a long history, as I recall.

DR. GEVANTMAN: It is now funded by OSRD. An important development is that we will go directly from the data on tape to printing of the book. The first volume of this book is anticipated within the next six months, and the second volume soon thereafter. Most of the difficulty in getting the book out has been in programming the material that has been compiled in a way to run smoothly from the tape directly to the final printing.

QUESTION: May I ask another general question. How often do you re-evaluate the priorities suggested by advisory committees both in your area and other areas?

DR. GEVANTMAN: In the past we have not re-evaluated frequently, largely because for financial reasons we haven't been able to implement the recommendations that we have. If we had been able to develop the program aggressively to a level three to five times what it is now, we probably would have had a number of re-evaluations of where we stand and needed priorities and needs for new work. Since the program has moved slowly, we have been forced to move slowly with the panels as well.

DR. SCHULMAN: To what extent have there been requests for special compilations in certain areas? That seems to me the type of correspondence that would help in evaluation of your priorities.

DR. GEVANTMAN: We have made a survey of the members of the American Chemical Society, inquiring what compilations they would like to have, and a large list resulted. The number of spontaneous requests that come in for special compiations is very small. There may be a few, but I am not aware of them.

DR. WADDINGTON: I would point out something that one or two of you mentioned. This morning, Dr. Rossini stated that at the CODATA Conference in Germany last summer, there was a suggestion from the USSR that there should be a study made of a program for compiling data of chemical kinetics. This idea is enthusiastically supported by Professor Kondratiev of the USSR Academy of Sciences who is currently the President of IUPAC. This is a complex and large area and there sill have to be very careful discussion about the magnitudes and nature of the programs to be conducted in a given country. It is definitely an area for international coordination.

QUESTION: In your solid state activities, have you taken any advantage of the material that is issued by the DOD-sponsored EPIC program?

DR. GEVANTMAN: That is one of the types of uncritical data compilation that was mentioned.

DR. BRADY: The EPIC program is an attempt as far as I can determine simply to extract information from the literature. There is little critical evaluation involved.

QUESTION: I would like to add a word, if I could, about the subject of priorities. We have been complaining all afternoon about the lack of funds and the resulting restrictions. It has one blessing. If you have a great many high priority things to do, and much less than enough money to do them with, it makes the choice simpler. You pick an obviously good one, and if you must choose between two good ones and you can only do one, you do the one that is easier to start. We're nowhere near the area where we are coming up to almost impossible situations of "Should we now go to the lesser priorities, or should we give more money to the high priority things." It saves a few headaches.

DR. BRADY: Before we break for coffee, I would like to bring up one thing.

Here in the audience there are a substantial number of people who are associated with the various data centers within the National Bureau of Standards.

At the coffee break and later, some of the members of the Advisory Board may want to discuss some of the programs with people who are representatives of these activities, so let me ask the people at NBS or who are associated with one or another of our data centers, to stand up and be recognized. (The individuals stood and were identified.)

(Recess for coffee)

DR. BRADY: We have now covered the areas of properties that are included in the program of the Office of Standard Reference Data. We will now discuss the other two broad categories we are interested in, that is, the data handling activities and information of the office, and then end our part of this afternoon's program with a presentation by Dr. Lee Kieffer of the Boulder JILA Center.

Mr. Joseph Hilsenrath who will speak on data systems development was a member of the Heat Division at the Bureau for several years prior to joining the Office of Standard Reference Data approximately a year and a half ago.

He is responsible for the development of Omni-Tab and a variety of other computer aids to processing of data, and has been developing some extremely flexible and adaptable systems lately within the purview of our office.

Note regarding composition of the following report:

The following pages which describe the work of the Data Systems Design Group of the Office of Standard Reference Data were reproduced from a typescript prepared on a Model 37 Teletype connected to a commercial time-shared computer service. In addition to the right-hand justified margins, the use of a computer permitted efficient editorial corrections.

DATA SYSTEMS DEVELOPMENT
By
JOSEPH HILSENRATH

As Dr. Brady mentioned, I represent the Data Systems Design Group in the Office of Standard Reference Data. It is a relatively small group, of which the productive members are Mrs. Carla Messina, Robert C. Thompson, and a few students from time to time.

Our work can be divided into three general areas: The preparation of general-purpose computer programs for numerical data reduction and file manipulation; for text editing and report generation; and last, but not least, for computerized typesetting.

We also assist the NBS Office of Technical Information and Publications in the computerization of the NBS Publication program which is extensive. We have produced about 20 items ranging from conference proceedings to individual research papers. These publications listed in Appendix A-1 were produced not by a single method but from a variety of sources and techniques. Some of the tabular material came from existing punched cards or existing magnetic tapes which were transformed by our programs to conform to specifications of various GPO typesetting programs. Other publications were keyboarded on a variety of terminals by the secretarial staff of the originating Divisions. Still others were produced at the GPO directly from magnetic tapes formatted by the authors themselves from instructions supplied by our group.

One item in the list merits special attention. That is the Index to the publications of the NBS Staff for the years 1966-1967. The word index here is really a misnomer as the book contains, for each publication, the authors; the title; the journal, volume, year, and inclusive pages; a full abstract; and a list of key words under which the work is indexed. In view of the above it would seem more appropriate to call this book an abstract journal. Figure 1 shows a number of typical abstracts as they will appear in the published volume and as they were keyboarded. The keyboarding was done on a typewriter-like terminal (an IBM 2741) connected to a time-sharing computer (IBM 1440) over a telephone line (via a 103A Data phone) without bothering with paper tape or magnetic tape. The text was subsequently edited and corrected at the terminal. After proofreading, the text was transfered from the computer disc to a

9335. Production and reaction of atomic fluorine in solids. Vibrational and electronic spectra of the free radical HNF, M. E. Jacox and D. E. Milligan, J. Chem. Phys. 46, No. 1, 184-191 (Jan. 1, 1967).

Key words: F atom reactions; force constants; HNF; HNF2? infrared spectrum; matrix isolation; NF; NF2? thermodynamic properties; visible-ultraviolet spectrum.

The species H]4NF, H]5NF, and D]4NF have been produced in an argon matrix at 14 °K by the reaction of photolytically produced atomic fluorine with NH. Sufficient concentrations of these species have been obtained for direct detection of two vibrational fundamentals, appearing at 1000 and 1432 cm)1 for H]4NF, as well as of an electronic transition between 3900 and 5000 Å involving a progression in the upper state bending frequency. Force constants and thermodynamic properties have been derived for HNF. Other species observed in these experiments include NF, NF2? and HNF2? Evidence is presented indicating that the hydrogen atom can be abstracted from HN3 by atomic fluorine.

9336. Physiological optics ... B. Judd, Appl. Opt. 6, No. 1, 13-

Key words: Color; glo... etry; physiological optics; psychoph...

Published work in phys... u of Standards is summarized und... -dark patterns, light measurement, ... and color perception. The bear... f the American Society of Testing an... ering Society, and of the American ... tions of the International Commissio... poses and methods of current work ar...

9337. Vacuum ultraviolet s... L. J. Padziemski, Jr., and K. L. And... 1-915 (July 1966).

9335. **Production and reaction of atomic fluorine in solids. Vibrational and electronic spectra of the free radical HNF**, M. E. Jacox and D. E. Milligan, *J. Chem. Phys.* **46,** No. 1, 184-191 (Jan. 1, 1967).

Key words: F atom reactions; force constants; HNF; HNF_2; infrared spectrum; matrix isolation; NF; NF_2; thermodynamic properties; visible-ultraviolet spectrum.

The species $H^{14}NF$, $H^{15}NF$, and $D^{14}NF$ have been produced in an argon matrix at 14 °K by the reaction of photolytically produced atomic fluorine with NH. Sufficient concentrations of these species have been obtained for direct detection of two vibrational fundamentals, appearing at 1000 and 1432 cm^{-1} for $H^{14}NF$, as well as of an electronic transition between 3900 and 5000 Å involving a progression in the upper state bending frequency. Force constants and thermodynamic properties have been derived for HNF. Other species observed in these experiments include NF, NF_2, and HNF_2. Evidence is presented indicating that the hydrogen atom can be abstracted from HN_3 by atomic fluorine.

9336. **Physiological optics at the National Bureau of Standards,** D. B. Judd, *Appl. Opt.* **6,** No. 1, 13-26 (Jan. 1967).

Key words: Color; gloss; light; perception of color; photometry; physiological optics; psychophysics; scaling of

Figure 1. A phototypset sample column from the volume of abstracts of publications of the NBS staff has here been superimposed on a typeout on the computer terminal of the text as it is stored on the computer. In this system tab positions and the overstruck characters signal a variety of actions to the typesetting system as follows:

a. the two tabs in front of the item number cause material following to be set in bold face type until instructed otherwise.
b. when a character is overstruck with the degree mark, the normal roman type face is called for.
c. a strike over sith the / (solidus) turns on the italics face.
d. a strike over the " (double quote) gives bold face as in a. above.
e. a strike over with the - (hyphen) gives a greek character corresponding to the latin alphabet.
f. a strike over with the] (right bracket) gives superscripts.
g. a strike over with the ((left parentheses) gives subscripts.

magnetic tape. The tape was delivered by messenger to NBS where it was processed on the NBS UNIVAC 1108 by a multiple-table insert program written by Robert C. Thompson a member of the Data Systems Design Group. The magnetic tape resulting from the pass on the UNIVAC 1108 is in the precise format and contains the numerous flags required by one of the automatic typesetting systems at the Government Printing Office.

Among the noteworthy features of this system are that the typist indicates by means of a system of overstrikes, which characters are to be greek, which are to be bold face, which are italics, and more particularly, which are subscripts and which are superscipts. The resulting product makes no compromise with notation. Greek letters actually appear as such, not as "gamma" or "beta", and subscripts and superscripts appear in inferior or superior positions as if set by hand.

Another interesting feature of this system is that the magnetic tape produced for typesetting is also used for the generation of an author index and a keyword index.

The foregoing discussion pertains to typesetting of material which had not previously been in computerized form. For material which is already on punched cards or computer tapes, we have written two other programs for typesetting. They are called TYPSET and KWIC. We illustrate first the results of the latter program.

Those of you who have used computerized files are undoubtedly familiar with permuted title indexes. These are reproduced by photographing computer printout, and hence often leave a great deal to be desired in the way of readability.

Our first solution to this problem is shown in figure 2. While the typesetting was sucessful, the product fell far short of what we expected. There did not seem to be sufficient gain in readability to warrant the added expense and normal delays incurred in phototypesetting. It would appear that material set in all capital letters is difficult to read even when printed quite clearly. Some improvements in readability was achieved through increasing the "letter spacing" - increasing slightly, the space between the letters.

It was at this point that Mrs. Messina volunteered to expand the program KWIC by combining it with an existing program called SUBSTITUTE which can replace any string of characters by any other string. Figure 3 shows the result of the program we call KWIC which takes a KWIC index stored in all caps and converts it to a highly readable form with proper capitalization. This transformation is achieved in large measure via a series of substitutions which treats all letters as lower case except those preceeded by a space. Still other exceptions: like articles which are not capitalized at all, or such words as USA or IBM, which

6623815	NOLOGY, CAMBRIDGE, MASSACHUSETTS ANNUAL REPORT NO 1	**/99MASSACHUSETTS INST. OF TECH CAMBRIDGE, OPERATIO	6623815
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6724014	Y COMPUTER AIDED INDEXING OF A SCIENTIFIC	ABSTRACTS JOURNAL BY THE UDC WITH UNIDEX. A CASE STUD	6724014
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6623825	ICAL LITERATURE. COMPUTER TECHNOLOGY COMPILATION OF	ABSTRACTS. REPORT NO 7 /FOREIGN SCIENTIFIC AND TECHN	6623825
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5709114	1957 REPORT OF PROJECT MICHIGAN.	ACOUSTICS AND SEISMICS. PERIOD 1 JUNE 1956 TO 1 MARCH	5709114
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6723892		AEROSPACE MEASUREMENT TECHNIQUES	6723892
6409054	SONAL TELEMETRY SYSTEM VALIDATION OF THE	AEROSPACE MEDICAL RESEARCH LABORATORIES 3-CHANNEL PER	6409054
6724050	BIBLIOGRAPHY WITH INDEXES	AEROSPACE MEDICINE AND BIOLOGY. A CONTINUING	6724050
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Figure 2. A portion of a KWIC index photocomposed from a regular print tape modified by an early version of the KWIC program. The legibility of the result is not much improved by the photocomposition process.

Thermal Conductance Factors for Preformed	Above-Deck Roof Insulation (1955)	USC	R257
Grading Of	Abrasive Grain for Grinding Wheels (1965)	USC	CS271
Grading Of	Abrasive Grain On Coated Abrasive Products (1967)	USC	PS8
Coated	Abrasive Products (1955)	USC	R89
Grading of Abrasive Grain On Coated	Abrasive Products (1967)	USC	PS8
(1965) Acrylonitrile Butadiene Styrene	ABS Plastic Drain, Waste and Vent Pipe and Fittings	USC	CS270
Acrylonitrile Butadiene Styrene	ABS Plastic Pipe (SDR PR and Class T) (1963)	USC	CS254
Rigid	ABS Plastic Pipe, IPS Dimensions (1959)	USC	CS218
Colors for Kitchen	Accessories (1938)	USC	CS62
Colors for Bathroom	Accessories (1938)	USC	CS63
Stove Pipe And	Accessories (1942)	USC	R190
Metal Lath Expanded and Sheet and Metal Plastering	Accessories (1960)	USC	R3
	Accoustical Materials (1960)	USC	R262
Solvent Welded Swp Size Cellulose	Acetate Butyrate Pipe (1957)	USC	CS206
Girls, and Boys Knit Underwear Exclusive of Rayon,	Acetate, and Nylon (1955) Infants, Childrens,	USC	CS198
waste and Vent Pipe and Fittings (1965)	Acrylonitrile Butadiene Styrene ABS Plastic Drain,	USC	CS270
PR and Class T) (1963)	Acrylonitrile Butadiene Styrene ABS Plastic Pipe (SDR	USC	CS254
Hollow Metal Single	Acting Swing Doors, Frames and Trim (1928)	USC	R82
	Adhesive Plaster (1952)	USC	R85
Water Resistant Organic	Adhesives for Installation of Clay Tile (1952)	USC	CS181
Polystyrene Plastic Wall Tiles, And	Adhesives for Their Application (1950)	USC	CS168
Chasers for Self Opening And	Adjustable Die Heads (1929)	USC	R51
Hot Dipped Galvanized Ware Coated	After Fabrication (1959)	USC	CS161
Wire Diameters for Mineral	Aggregate Production Screens (1942)	USC	R147
Coarse	Aggregates, Crushed Stone, Gravel, and Slag (1948)	USC	R163
Polyethylene Sheeting Construction, Industrial And	Agricultural Application (1961)	USC	CS238
(1942)	Agricultural Insecticide and Fungicide Packages	USC	R41
Packaging of First	Aid Unit Dressings and Treatments (1941)	USC	R178
Packaging Of	Air Brake (Electric Railway) Parts (1935)	USC	R162
Tank Mounted	Air Compressors (One-Fourth to 10 Horsepower (1948)	USC	R202
Tank Mounted	Air Compressors (1956)	USC	CS126
Pipes, Ducts and Fittings for Warm Air Heating And	Air Conditioning Systems (1960)	USC	R207

Figure 3. A portion of a phototypeset Key Word In Context index produced from an existing output tape. The KWIC program converted to initial caps and lower case all but a limited number of articles and connectives. Note that ABS, SDR, PR, and IPS appear in all caps as required. Figure 4 shows a portion of the substitution table which was read in to achieve these transformations.

should appear in all caps, are also handled in a simple and straightforward manner. These transformations are achieved via a substitution table of which a portion is shown in figure 4.

Interestingly enough, the program intended originally for KWIC indexes, was easily modified to provide a very useful typesetting program for program listing, where the letters must appear as capitals. Figure 5 shows a portion of a listing of a program run through our TYPSET program and set at the Government Printing Office on a Linofilm machine using the Times Roman type face. Here again the variable width letters so characteristic of graphic arts quality printing is a distinct drawback.

A dramatic improvement in clarity and readability is achieved simply by changing to a mono-width type face such as is found on an ordinary typewriter. Figure 6 shows a portion of a program listing run through TYPSET and set at the GPO as before, but using the Clarinda Typewriter font. Although less aesthetically pleasing to some, this type face seems to be the ultimate in clarity for program listing and indeed for much of what comes off the computer.

The program discussed heretofore for typesetting are more properly called "insert programs" as they prepare a magnetic tape by inserting into the character stream a variety of characters or character sets called "flags". These tapes do not drive the photounits. They are further transformed by programs at the GPO which are more properly called typesetting programs. It is the tapes resulting from the GPO programs which drive the photounits.

One of our programs is an honest-to-goodness typesetting program. It generates a magnetic tape which drives the new Linotron machine at the GPO directly. Figure 7 shows references produced by Dr. Garvin's Chemical Kinetics Data Center at NBS and its typeset version produced on the Linotron by a program, written by Mrs. Messina, which converts magnetic tape written in the General Purpose Scientific Document Image Code (GPSDIC) to one which will drive the Linotron machine at the Government Printing Office.

The General Purpose Scientific Document Image Code

Two of our data centers at NBS, the Chemical Thermodynamics and the Chemical Kinetics Data Center, have provided the motivation for a very comprehensive and forward looking computer system which is designed to handle text material of the complexity, which is so characteristic of chemistry and chemical documentation.

That work, which is done by Dr. Blanton C. Duncan and Dr. David Garvin, has led to the development of a general purpose scientific document image code and a comprehensive package of computer programs in support thereof.

```
$ *
 IEND = $   IGN = *
 IA = ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789                     A><
 IB IS
                                                                                $
 IEND = $   IGN = *
 IA = ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789                     A><
 IB IS  ******                                          U. S. DEPT. OF COMMERCE
******                                         U. S. DEPT. OF COMMERCE STANDARD
 IEND = $   IGN = *
 IA = ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789                     A><
 IB IS  **********************                                    TITLE WORD INDEX
**********************                                      TITLE WORD INDEX$
 IEND = $   IGN = *
 IA = ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789                     A><
 IB IS  FINIS$
FINIS$
ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789'/(*)=,$.+
 0 6 3
   0>< 0
   0>< 1
/(SDR/                                   /(>S>D>R/
/(P/C)/                                  /(>P>V>C)/
/(PE)/                                   /(>P>E)/
/ PR)/                                   / >P>R)/
/ PR /                                   / >P>R /
/ SDR/                                   / >S>D>R/
/ DWV/                                   / >D>W>V/
/ IPS/                                   / >I>P>S/
/ ABS /                                  / >A>B>S >/
```

Figure 4. A portion of a substitute table which is read in a run time by the KWIC typesetting program in order to achieve the transformation shown in the last figure.

```
C     READ. PRINT. PUNCH ARE THE UNIT NUMBERS FOR THE CARD READER.
C     PRINTER. AND CARD PUNCH
C     LCOL IS THE COLUMN IN WHICH THE CARD TYPE LABEL IS PUNCHED
C     IF IT IS ZERO. TYPING IS DONE BY ORDER OF APPEARANCE (FIRST CARD
C     IS TYPE ONE. AND SO ON)
      READ (READX,10) ,NCIN,NCOUT,READ,PRINT,PUNCH,LCOL,IWIDTH
C     IF THESE SPECIFICATIONS ARE BLANK. DEFAULT VALUES ARE TO BE
C     ASSIGNED
      IF (READ.EQ.0) READ=READX
      IF (PRINT.EQ.0) PRINT=PRINTX
      IF (PUNCH.EQ.0) PUNCH=PUNCHX
      IF (IWIDTH.EQ.0.OR.READ.EQ.READX) IWIDTH=80
      WRITE (PRINTX,40) ,READ,PRINT,PUNCH
      IF (PRINT.NE.PRINTX) WRITE (PRINT,40) ,READ,PRINT,PUNCH
C     COLUMN 80 OF THE FIRST CARD (THE LIST OF VALID CHARACTERS)
C     CONTAINS A CHARACTER USED AS A STRING TERMINATOR
      STOP=ALPHB(80)
C     COLUMN 79 OF THIS CARD IS BLANK
      SPACE=ALPHB(79)
      WRITE (PRINT,25) ,(ALPHB(J),J=1,80)
      WRITE (PRINT,30) ,NCIN
```

Figure 5. A portion of a computer listing phototypeset from a FORTRAN program deck which was transformed by the program TYPSET. The readibility of this listing is somewhat impaired by the variable width of characters so characteristics of graphic arts quality type faces. See Figure 6 for a much more readable product.

```
          IF (L-J) 80,70,90
    70    IF (K) 80,120,80
    80    WRITE (IOTAPE,280)
          GO TO 150
    90    IF (IA(83)-IA(85)) 80,100,80
   100    K=2*(L/2)-LA
          IF (K) 110,120,110
   110    IW=IW+1
          IB(IW)=IA(85)
   120    J=1
   130    IF (IB(J)-IA(83)) 140,160,140
   140    J=J+1
          IF (J-(IW+1)) 130,150,150
   150    RETURNI
   160    IF (IB(J+1)-IA(85)) 190,170,190
   170    J=J+2
          DO 180 I=J,IWA
   180    IB(I-1)=IB(I)
          GO TO 220
```

Figure 6. A portion of a computer listing phototypeset from a FORTRAN deck which was transformed by the program TYPSET. In this case use was made of a monowidth type face (CLARINDA TYPEWRITER) on the phototypesetting machine.

LOCAL FILE NO.		BRIEF REFERENCE	CENTRAL FILE NO.
BRIEF: DG/1921	Page 1	BBPCA-1966-70-664	CKIC/10623

AUTHOR(S)

AUTH: Grabke, H. J.

TITLE

TITLE: Zur Kinetiok der Reaktionen von Graphit mit CO2 -CO- und H2O-H2 -Gemischen

REF.	YR.	VOL.	NO.	PG.
REF: Berich. Bunsengesellschaft	1966	70		664

REACT: CO2 + C = 2 CO

H2O + C = CO + H2

O(ads.) + C = CO

INDEX: Experimental: gas: surface: Bond formation CO: oxidation: rate: tracer: chemisorption: surface-reaction: carbon-graphite: carbon-dioxide: carbon-monoxide: hydrogen-molecule: oxygen-atom: water:

REMARKS: ▣
REMARKS: ▣
REMARK: water vapor present in some cases:

Figure 7a

Sample typed input for the Chemical Kinetics Information Center literature reference file.

The copy shows several input conventions that are used by the computer program that transcribes the records. These are strike-overs to correct copy, the use of a special overstrike (◊) to delete a character, a special symbol (▣) to delete a line, and the slashing of characters to indicate that they are subscripts.

BRIEF: DG/1921 Page 1 BBPCA-1966-70-664 CKIC/10623
AUTH: Grabke, H. J.
TITLE: Zur Kinetik der Reaktionen von Graphit mit CO_2 -CO- und H_2O-H_2

-Gemischen
REF: Berich. Bunsengesellschaft 1966 70 664
REACT: $CO_2 + C = 2\,CO$

$H_2O + C = CO + H_2$

O(ads.) + C = CO
INDEX: Experimental: gas: surface: Bond formation CO: oxidation: rate: tracer: chemisorption: surface-reaction: carbon-graphite: carbon-dioxide: carbon-monoxide: hydrogen-molecule: oxygen-atom: water:
REMARK: water vapor present in some cases:

Figure 7b. The typeset version of the file card in figure 7a. The file card was typed on a tape-typewriter and coded in the General Purpose Document Image Code. A typesetting program prepared a magnetic tape which was used to drive the Linotron electronic typesetting machine directly.

Because of our successful typesetting work and for other reasons, I venture to predict that the document image code will shortly begin to exert an important standardizing function, in the data handling for various data centers.

We view the GPSDIC code as a most logical way for the various data centers to store data and text. Furthermore, for us it represents a neutral ground from which to go forward to automatic typesetting via a single through comprehensive program package. For the data centers the chore of converting to the Document Image Code will be miniscule if they adopt the practice of storing their information in the USASCII Code.

Time is available for only a brief description of the Document Image Code. It has a provision for indicating uniquely 188 different characters, Greek letters, subscripts, superscripts, and so on. Furthermore, the code convention permits one to indicate in the computer word itself whether that number or letter is on the line or that it is a subscript or a superscript. There is even room to indicate whether the characters are to be bold face or italics.

Figures 8 and 9 show the 188 characters around which the GPSDIC system is built and which will be available on an IBM printer. With this set of characters one can come off a computer printer with upper and lower case, with subscripts and superscripts and even Greek letters. We expect to use the computer printer as a galley, and when that is letter perfect, then, and only then, would the tape be sent forward for typesetting. Thus, we will avoid the copy editing and most of the proofreading at the galley stage. We are convinced that a sound computer-assisted typesetting procedure will reduce considerably the cost and the delay in producing data tables.

The general-purpose document image code also has some special characters which will permit us to print on a line-printer (also on a typewriter-like input device) chemical structures and mathematical formulas.

The characteristics of input devices have in the past been a serious deterient and will in the future be an important ingredient in the development of more practical and more natural information and data systems. Figure 10 shows some material which one might suppose had originated on an ordinary typewriter. It was, in fact, produced on a new Model 37 Teletype. Had the Teletype been connected to a computer, as it can be, there would have been transmitted and stored all the information necessary to play this material back. At that time the computer would cause the paper to move a half-space backward for the superscripts and a half-space forward for the subscripts. The same machine will have an alternate typebox which will produce display formulas and chemical structures as is shown in figure 11.

0		16	0	32	@	48	P	64		80	p
1	!	17	1	33	A	49	Q	65	a	81	q
2	"	18	2	34	B	50	R	66	b	82	r
3	#	19	3	35	C	51	S	67	c	83	s
4	$	20	4	36	D	52	T	68	d	84	t
5	%	21	5	37	E	53	U	69	e	85	u
6	&	22	6	38	F	54	V	70	f	86	v
7	'	23	7	39	G	55	W	71	g	87	w
8	(	24	8	40	H	56	X	72	h	88	x
9	)	25	9	41	I	57	Y	73	i	89	y
10	*	26	:	42	J	58	Z	74	j	90	z
11	+	27	;	43	K	59	[	75	k	91	{
12	,	28	<	44	L	60	\	76	l	92	|
13	-	29	=	45	M	61	]	77	m	93	}
14	.	30	>	46	N	62	^	78	n	94	~
15	/	31	?	47	Ø	63	_	79	o	95	

Figure 8. These 94 characters of the GPSDIC code are in accord with those in the USASCII Standard. (Code for Information Interchange).

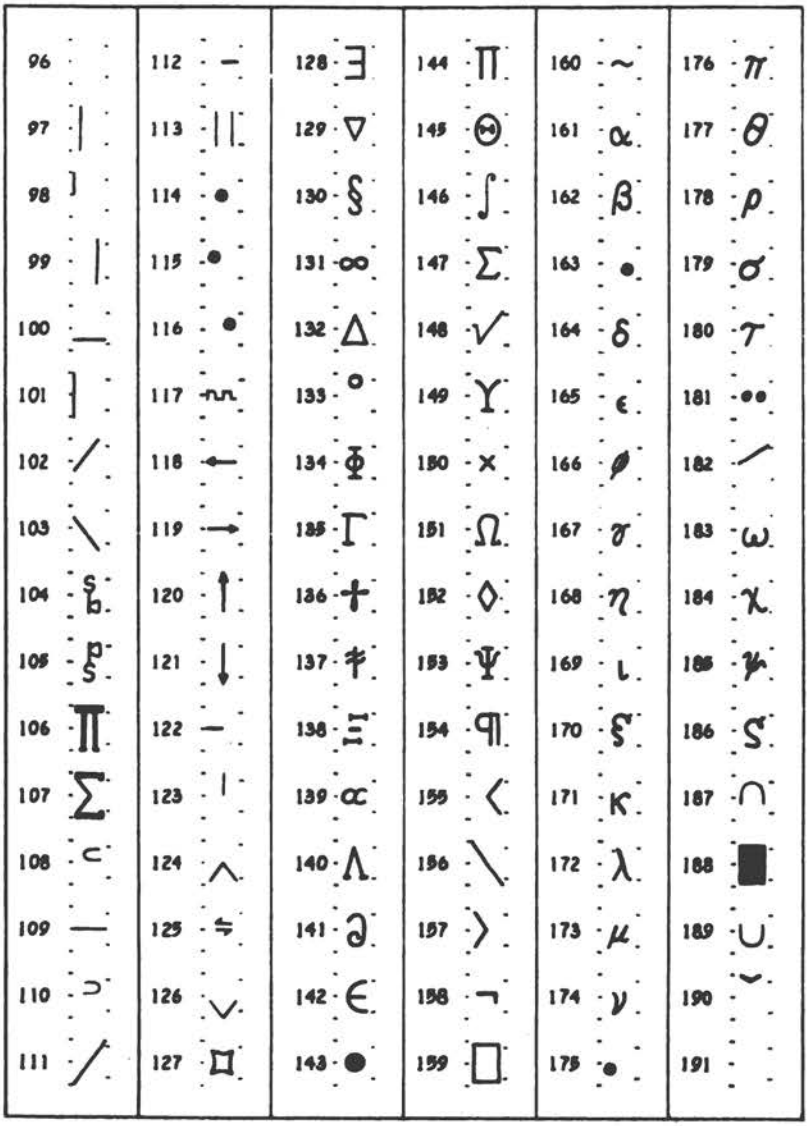

Figure 9. These characters of the GPSDIC code can be transmitted over regular communication lines by employing the shift-out feature of the USASCII Standard.

THIS IS A MODEL 37 SEND-RECEIVE SET
OPERATING AT 150 WPM.

The following will demonstrate the use of reverse line feed, fractional reverse line feed, line feed, and fractional line feed. With these features we may print mathematical expressions:

$$(a + b)^2 = a^2 + 2ab + b^2$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} \ldots\ldots\ldots$$

Using the "Shift-out" feature, we have an additional 32 printing characters available.

$$\frac{\alpha^2}{\xi^2} + \frac{\beta^2}{\xi^2 - 1} = \phi^2 \qquad (1 < \xi < \infty)$$

$$\cos^2\lambda - \sin^2\theta = \sin(\theta + \lambda)\sin(\theta - \lambda)$$

Hydrocarbon molecular structures may also be constructed:

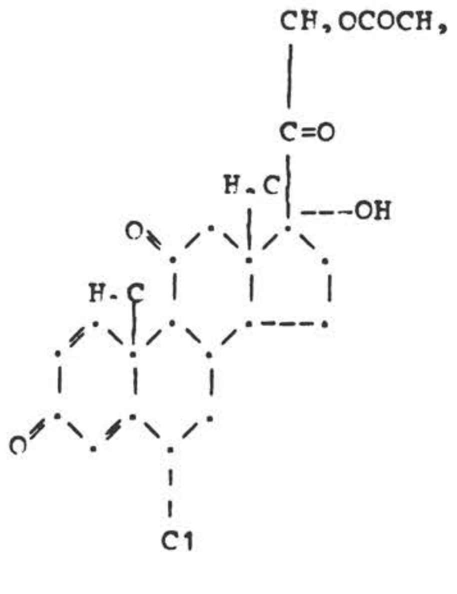

Figure 10. An example of the extent to which the new model 37 Teletype is able to handle the complex notation of mathematics and chemistry in computer readable form.

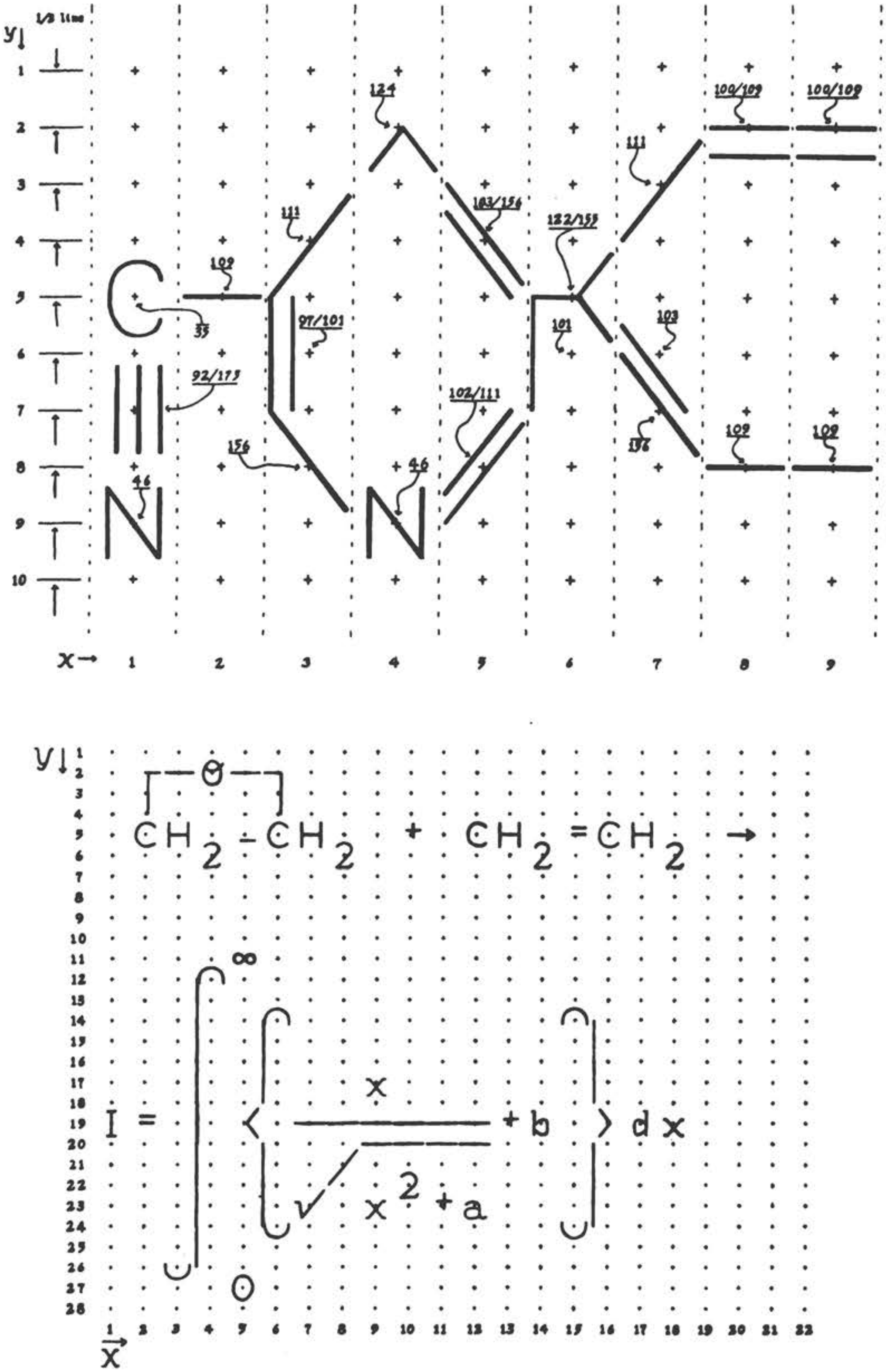

Figure 11. An example of the type of material which can be stored on a computer using the shift-out features of the USASCII Code.

The proliferation of such typewriter-like remote computer terminal will, in our view, revolutionize and simplify the storage and retrieval and interchange of the standard reference data with which we are so concerned.

The ability to input to a computer a complex mathematical formula in display form has two other important ramifications. The first is to computing and the second to typesetting. Klerer and May have written a compiler for the GE225 - a really small computer by todays standards - which recognizes such complex mathematical expressions and writes a program to evaluate them. In their system a computer program is simply a clear statement of the problem - nothing more and nothing less.

The advantage of such a system for computerized typesetting of complex mathematical formulas is equally great. This has not, yet, been recognized by those who have addressed themselves to the problem of computer-assisted typesetting of mathematical text, even though the work of Klerer and May was published in 1964 and a number of their predecessors published as early as 1961.

Remote Access to Standard Reference Data

Until now we have discussed batch mode computer operations. While such operations will continue to be part of the work of a data center, the time is ripe to plan for data systems designed for use via remote terminals over communications lines. The phenomenal growth of the time-shared computer industry in the short space of four years is ample evidence that remote use of computers is a reality that will have an important impact on the operation of data centers in the next few years.

A recently published survey of time-shared computer services shows 44 separate companies offering service in 23 states. Twenty companies offer services in the state of California, 13 in New York and Pennsylvania, etc. New companies offering this service are springing up almost weekly.

These computing services are used via typewriter-like terminals with conversational type instructions using the BASIC language which has now become a fairly standard means for communication with a time- shared computer. Our experience with BASIC as a computer language shows it to be very suitable for writing programs for retrieval of standard reference data. It was gratifying, therefore to hear from Dr. Fink that the ASTM has already stored a file of powder diffraction data on a time-shared computer.

The foregoing statistics; the nearly universal use of Dartmouth BASIC, or at most minor modifications thereof, as a programming language; the excellent file handling facility which the systems provide the user; and the economic aspects of time-shared computer operations, all argue for giving the commerical time-sharing computer industry a prominant role in the storage and retrieval of standard reference data.

One of the characteristics of time-shared computer systems merits some special attention. One often hears complaints that the program size and file sizes on these systems are limited. A limit of 6000 or so characters per program or 1200 data point does seem limiting for persons used to working with the large core memories so characteristic of present day computers operating in the batch mode. Our experience with a half dozen or so time-sharing systems operating on nearly as many machines, points to a contrary conclusion so far as their application to computerization of standard reference data is concerned. One does not read every item in every drawer of a card file when searching for information on zebras. One goes directly to the drawer marked "z". It is no less sound to subdivide files for computer storage than it is in an ordinary card catalogue. The economic stakes are, if anything, much higher in file organization on a computer disc than they are in a well organized library card catalogue. The data bases we will be concerned with in the next few years can easily be accommodated by the present commercially available systems both from an economic as well as a utilitarian view.

No amount of segmentation of data files can, however, remove the need to choose which data are worth storing on a computer and which are not. In most practical cases which we have thus far considered, the choices seemed clear cut. We should store around the clock: the fundamental physical constants, the atomic weights of the elements, critical temperatures and pressures, boiling points, melting points, heats of fusion and vaporization, heats of formation, ionization potentials, etc.

All of these data were published somewhere, some (like the physical constants) have been printed on wallet size plastic cards which many of you may indeed be carrying. Why then should one need to call a computer for the data? To make sure that the values are the latest and best. How else can one be sure he has not missed one or more revisions?

Obviously, the computer-stored data will not be any more up-to-data than the reprint in your files unless the organization supplying the data makes a special effort to update the files as often and as promptly as the situation demands it. This would indeed be the case if the Office of Standard Reference Data were to undertake the systematic collection and dissemination of such computerized data bases.

We see less profit in storing for remote access, atlases of spectral lines, or detailed listing of atomic energy levels. These are more properly handled on magnetic tape. Nor do we see a need for storing Einstein or Debye tables which can so easily be computed when needed. In the latter case the system will provide easy means for extracting fundamental vibrational frequencies for polyatomic molecules to feed into the Einstein code or Debye Thetas to feed the Debye code to obtain computed specific heats or other thermodynamics properties.

Figures 12 and 13 show the results of two types of data retrieval programs. The first contains the ionization - potentials for the single ionization of those atoms in the periodic table for which data have been reported. The program (IPONE) is quite specialized in that it only provides a single value for a single element - one at a time. The second program (PFRIOD) is more general. It provides a dozen or more facts about each of the elements of the periodic table. The program is open ended as other data can easily be added. These programs are only illustrative of the variety of ways in which a data base can be extracted from a computer via a remote terminal.

Feedback is an important ingredient of a viable computer-based data retrieval system. It so happens that the file generation features of most of the time-shared programming systems provide a mechanism for a fairly automatic reporting system for data file use by accredited users.

It is possible in most versions of BASIC to incorporate in a search program a few instructions which will write on one or more "saved files" or logs. Not only can the system keep a record of who used a particular file but it can also record the question that was asked, and even the answer that the program delivered.

My time is too short to go into any more detail, but this will give you an idea of the kind of interesting problems that we are involved in.

DR. BRADY: A few questions?

MR. HILSENRATH: If any of you would like to see some sample of the kind of material that has been typeset, you are welcome to look.

DR. BRADY: It is probably hard to ask a short question about this stuff, but these techniques are of tremendous flexibility and applicability to almost anything we are doing.

QUESTION: If you lived in Montana, how could you get on the line, long distance?

MR. HILSENRATH: The information you seek has to be worth the cost of the long distance call. If it is, then there is no problem. If it isn't, then you don't make the call. If you were investing a good deal of time in calculations involving many molecular weights which were last revised in October of 1961,

```
IPONE      11:05    CEIR    01/29/69

IPONE GIVES THE IONIZATION POTENTIALS
IN ELECTRON VOLTS FOR THE NEUTRAL ATOMS.
RESPOND TO ? WITH AN ATOMIC NUMBER.?18

THE IONIZATION POTENTIAL FOR THE ATOM
WITH ATOMIC NUMBER Z =  18   IS  15.755   E.V.


TYPE A VALUE OF  Z OR A ZERO TO QUIT.?90


DATA FOR THE RARE EARTHS ABOVE
Z=90 HAVE NOT BEEN REPORTED.

TYPE A VALUE OF  Z OR A ZERO TO QUIT.?57

DATA FOR THE RARE EARTHS [Z=58 TO 71]
HAVE NOT BEEN REPORTED.

TYPE A VALUE OF  Z OR A ZERO TO QUIT.?87

THE I.P. FOR FRANCIUM [Z=87] IS NOT REPORTED.

TYPE A VALUE OF  Z OR A ZERO TO QUIT.?0

          * * * *
NOW THAT YOU HAVE THE DATA,
YOU SHOULD HAVE A REFERENCE.
IF YOU WISH MORE INFO ON THESE
DATA,TYPE A ONE,IF NOT TYPE A ZERO.?1
.
        ****************
 DATA ARE FROM 'ATOMIC ENERGY LEVELS'
VOL.3 BY C.E.MOORE. NBS CIRCULAR 467.
PUBLISHED IN 1958. THE I.P. FOR SI
IS TAKEN FROM NSRDS-NBS 3,SECT. 2
'SELECTED TABLES OF ATOMIC SPECTRA
ATOMIC ENERGY LEVELS AND MULTIPLET TABLES SI I'
BY C.E.MOORE PUBLISHED NOV. 30,1967.

THE PROGRAM 'NSRDS' CONTAINS A
LIST OF OTHER PROGRAMS IN THIS SERIES.

*** ONE WORD OF CAUTION***
IF THE NUMBER ON THE LAST LINE
IS NOT EXACTLY 641.957, SOME OF
THE ABOVE ANSWERS MAY BE IN ERROR.
THE SUM OF THE STORED DATA IS 641.957
```

Figure 12. A record of a session at a model 33 Teletype connected to a time-shared computer on which was stored a small program (3200 character) containing the first ionization potentials for certain atoms. As this BASIC Compiler does not have the "string variable" feature, questions are answered via numbers. The numbers circled are the users responses.

```
PERIOD    16:52    UOM  BASIC    16 JUN 68


THIS PROGRAM GIVES THE PROPERTIES OF THE
ELEMENTS. TYPE EITHER THE NAME OR THE
THE SYMBOL FOR THE ELEMENT.? H


HYDROGEN WAS DISCOVERED IN  1776  BY CAVENDISH
ATOMIC WEIGHT IS  1.00797 ,ITS VALENCE IS 1
DENSITY =  .08375 KG/METER CUBED
THE ELECTRON CONFIG. OF THE GROUND STATE  IS -- IS 2S1/2 --
THE IONIZATION POTENTIAL IS  13.595 ELECTRON VOLTS.
THE STRONGEST SPECTRAL LINE IS  1215.66  ANGSTROMS.
    * * LOW LYING ATOMIC ENERGY LEVELS * *
2J+1               LEVEL              2J+1              LEVEL
 2                  0                  8                 82259   *
 18                 97492              32                102823  *
THE CRYSTAL FORM IS HEX.C.P.
THE DISTANCE OF CLOSEST APPROACH IS  .92 CRYS.ANGS.
M.P. = -259.400  B.P. = -252.700  DEGREES C.
HEAT OF FUSION =  15  CAL/G/DEG C
MOLAR HEAT CAPACITY AT 298.15 DEG K =  6.89

* * * NOTE * * *
A CRYSTAL ANGSTROM =(KA) = A/1.0020
THE ATOMIC ENERGY LEVELS ARE GIVEN IN WAVE NUMBERS.
MOST OF THE LEVELS HAVE BEEN AVERAGED.
MORE DETAILED INFO WILL BE ADDED LATER.
```

Figure 13. shows the results from an experimental program designed to illustrate how easy it is to extract information from a data file using the Basic Programming language. The circled material was stored systematically in the data file and printed out by the program which had access to the data file. Other programs may extract different portions of the data or arrange the information in a different order. Present systems permit a program to draw information from as many as six different files. The program to produce this figure is shown in the figure 14.

```
70 DIM D(50,13)
80 PRINT'THIS PROGRAM GIVES THE PROPERTIES OF THE'
82 PRINT'ELEMENTS. TYPE EITHER THE NAME OR THE'
84 PRINT'THE SYMBOL FOR THE ELEMENT.';
90 INPUT A$
91 IF A$ = 'STOP' THEN 160
92 PRINT
98 LET R=2
99 LET C= 13
100 FOR I= 1 TO R
110 READ E$(I),S$(I),G$(I),D$(I),Y(I)
111 READ F$(I),V$(I),M(I),B(I),L(I),C(I)
120 FOR J= 1 TO C
130 READ D(I,J)
140 NEXT J
142 IF A$ = E$(I) THEN 500
144 IF A$ = S$(I) THEN 500
150 NEXT I
155 PRINT' DATA FOR ';A$;' HAVE NOT YET BEEN ENTERED.'
160 STOP
500 PRINT E$(I);' WAS DISCOVERED IN ';Y(I);' BY ';D$(I)
504 PRINT'ATOMIC WEIGHT IS ';D(I,1);',ITS VALENCE IS ';V$(I)
506 PRINT'DENSITY = ';D(I,2);'KG/METER CUBED'
510 PRINT'THE ELECTRON CONFIG. OF THE GROUND STATE ';
511 PRINT' IS -- ';G$(I);' --'
512 PRINT'THE IONIZATION POTENTIAL IS ';D(I,4);'ELECTRON VOLTS.
514 PRINT'THE STRONGEST SPECTRAL LINE IS ';D(I,5);' ANGSTROMS.'
516 PRINT'     * * LOW LYING ATOMIC ENERGY LEVELS * *'
517 PRINT'2J+1','LEVEL','2J+1','LEVEL'
518 PRINT D(I,6),D(I,7),D(I,8),D(I,9);' *'
519 PRINT D(I,10),D(I,11),D(I,12),D(I,13);' *'
520 PRINT 'THE CRYSTAL FORM IS ';F$(I)
521 PRINT'THE DISTANCE OF CLOSEST APPROACH IS ';D(I,3);'CRYS.ANGS.'
530 PRINT'M.P. = ';M(I);' B.P. = ';B(I);' DEGREES C.'
532 PRINT'HEAT OF FUSION = ';L(I);' CAL/G/DEG C'
534 PRINT'MOLAR HEAT CAPACITY AT 298.15 DEG K = 'C(I)
600 PRINT
900 PRINT'* * * NOTE * * *'
910 PRINT'A CRYSTAL ANGSTROM =(KA) = A/1.0020'
912 PRINT'THE ATOMIC ENERGY LEVELS ARE GIVEN IN WAVE NUMBERS.'
914 PRINT'MOST OF THE LEVELS HAVE BEEN AVERAGED.'
916 PRINT'MORE DETAILED INFO WILL BE ADDED LATER.'
918 PRINT
999 GOTO 90
```

Figure 14. This program produced the output in the previous figure.

could you be really sure that no changes have been published since that time? That information certainly is worth a few dollars in a long distance call. The commercial time-shared computer companies are so enterprising that before long there won't be any need to make a long distance call. If there is enough technical activity in an area, they will put in a foreign exchange line or something equivalent which will get you the information via a local call.

QUESTION: This going over leased wires is fairly slow at this point, and we could need a lot of information out here. Do you see any break in that bottleneck?

MR. HILSENRATH: Well, if you need a lot of information then you probably don't want to have it come over a telephone line. If you have volumes of information, you should have a system where it could be sent to you airmail, or something of that kind. There is a whole spectrum of problems. Some can be solved very readily by teletype and others cannot.

QUESTION: I just wanted to comment that it seems to me it would be a lot more profitable to work on a rapid printing system rather than central storage, requiring data to go to the vast number of people who are involved from the computer center, even though now and for a relatively long time in the future a comparatively small number of people are going to have access. If you want to ask a question, you want the answer now, not tomorrow or the next day.

MR. HILSENRATH: Well, you say a relatively small number of people. There are 40 companies, and my guess is that they have 100 customers each, so there are 4000 terminals at the very least. This number will probably double next year.

QUESTION: I recognize that, but it is still a very small number of people concerned with this information who would want access to it.

MR. HILSENRATH: Oh. Well, I should have prefaced my remarks by saying that I believe the printed book is here to stay for a long, long time. The printed book will still be a major part of us and so will the reprint, so I am not suggesting that this is the only mechanism. But I am suggesting that there are many applications where it is nice - even important - to be able to dial the computer and get an immediate answer to a specific data question.

I am not suggesting that this is a solution to all the data problems. As a matter of fact, in a small town, if 10 people have terminals and they all try to get on a long distance line, they will tie up the switchboard for the whole city. So I am not saying that all of the problems are solved. A great deal more has to be done in the matter of communication services, but there are people working in directions which should cut communication costs down to one-hundredth of what it costs us now.

DR. BRADY: I think probably we ought to proceed on to the next presentation, which is by Dr. Herman Weisman, who is in charge of the Information Services activity of the Office of Standard Reference Data.

INFORMATION SERVICES

By

Dr. Herman M. Weisman

DR. WEISMAN: Thank you, Dr. Brady.

Mission - To provide the services to the technical community that are determined to be useful and to maintain the collection of data that constitutes the data center at the National Bureau of Standards -- indexing, storing, and retrieving data as required. *

Functions of the Information Services - In order to fulfill the stated mission, the Information Services sees itself as having four basic units of activities. These units are (1) Data File, (2) Compilation and Editorial Services, (3) Inquiry Services, and (4) Analysis and User Relations.

Specific Activities of Each Functional Unit - Data File - The Data File collects, maintains, and stores data, information, and documents of pertinence to the entire NSRDS. Inherent in its objective is the analysis, classification and indexing of all items in the File. Inherent also is the system of data, information, and document retrieval, as well as the provision for periodic accession lists, bibliographies, and indices as required or as desirable.

Compilation and Editorial Services - This unit's mission is to act as an editorial intermediary between technical data centers and other individuals and groups producing data compilations, on the one hand, and the publishers on the other hand. The publishers could be the Government Printing Office or commercial publishers. In its work with the Government Printing Office, it serves as an interface between the data compilation producers, and the NBS Office of Technical Information, to the Government Printing Office. Another of its functions is to produce the NSRDS News. It also is providing editorial resources for the production of various brochures describing the NSRDS, its data centers, and

*NSRDS-NBS-1, National Standard Reference Data System, Plan of Operation, by E. L. Brady and M. B. Wallenstein. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Price 15 cents.

publications. Among its long-range concerns will be information and data media other than publications, such as tapes, microfiche, etc.

Inquiry Services - This is the unit which provides coordinated services from the Data File, from the Compilation and Editorial unit of the Office, and from other sources in the NBS and the NSRDS associated data centers. It replies to queries received by the program, if they are within the capability or scope of the program. Sometimes inquirers are referred elsewhere, or reference sources furnished or copies of reference sources, or data compilations or other publications are provided.

Analysis and User Relations - This unit has the task of understanding the requirements, both present and future, of the NSRDS's actual and potential users. It has the responsibility of providing the Office with information on how best to meet user needs. Another task is to develop feed-back mechanisms to evaluate the services provided.

The limited financial resources of the Office of Standard Reference Data have imposed severe restrictions on Information Services. Necessarily, Information Services is operating on a caretaker and holding-on basis. At present, Information Services has one professional person with a secretary. Despite this penurious existence, Information Services has been able to function — in a limited way — and also to make some effective contributions to the program. Some of the contributions are:

Data File - The Data File has built up a very comprehensive collection of compilations of data in the physical sciences. It has within its library shelves and files the available world-wide data compilations containing more than 1200 documents, three-fourths of which are compilations and related works. It is also in the process of putting out an annotated accession list so that it can be revised painlessly. Lack of both personnel and other resources have prevented the Data File from indexing its holdings. It has in the past examined classification, indexing, and thesaurus problems so that when resources are available, the Data File can proceed into these activities.

Compilation and Editorial Services - The Compilation and Editorial Services has been responsible for the NSRDS News which many of you have seen. Copies of this newsletter are available. I have also passed to you a listing of the publications of the Office of Standard Reference Data which this unit has provided services from a very limited to an extensive way. In the past, it was involved in a substantial way in developing computer programming to obtain a mechanized means for standard reference data publications. The NBS development of the Taxywriter is an important step toward mechanization. Activities and mechanization are coordinated with the Data Design and Development Group. It will also play a role in commercial publication of NSRDS compilations which the NSRDS Act has made possible.

Inquiry Services -

Dec. 1, 1965 - Nov. 1966
Total Number of Inquiries - 119
Replies Available at OSRD - 68
Replies Available Within NSRDS - 12
Referral Elsewhere at NBS - 10
Referral to Other Sources - 21
Negative Replies - 8

Nov. 1, 1966 - Oct. 31, 1967
Total Number of Inquiries - 274, plus 145 requests via Nucleonics and Scientific Research

Replies Available at OSRD - 329
Replies Available Within NSRDS - 20
Referral Elsewhere at NBS - 8
Referral to Other Sources - 48
Negative Replies - 28

Nov. 1, 1967 - Oct. 31, 1968
Total Number of Inquiries - 299

Information Available Within OSRD - 209
Replies Available Within NSRDS Centers - 18
Referral Elsewhere at NBS - 16
Referral to Other Sources - 68
Negative Replies - 25

Analysis and User Relations - This unit has conducted several user-type studies. Among the first was an analysis of the American Chemical Society questionnaire which was sent out to the full 100,000 membership of the American Chemical Society. Approximately 16,000 replies were received. Overwhelmingly, response indicated that present compilations of data satisfied poorly, or at best only moderately, the requirements of the membership of the ACS. The survey identified the properties which ACS workers most often sought in the literature, as well as those compilations most often consulted by respondents. A number of worthwhile comments and suggestions were contributed on approaches to be taken, compilation priorities, and techniques of format and presentation.

In association with Industrial Research, a survey was conducted in one of the 1967 issues of the magazine to determine data and information needs of scientists and engineers within the industrial research community, how such needs are met, patterns of use of data, information, and reference sources, and what problems there were in finding required data and information. The results indicated that of about 600 scientists and engineers responding, 75 percent experienced problems in locating or obtaining materials properties data. During a typical week, 55 percent of the respondents must look up properties data from 1-5 times. Among others, the task is more demanding, occurring 6-10 times for 22 percent, and more than 10 times for 19 percent. Generally, it takes less than an hour for the majority to locate the necessary information; however, 24 percent spent from 1-8 hours, and 8 percent normally searched for days or weeks. Among other items of interest the survey revealed was that the printed book is the most frequently used and preferred medium form for data in use by respondents, and 72 percent of the respondents require and use bibliographies.

Very recently, another survey was completed — A Pilot Study for Determining Technical Reference Data Use Patterns of NBS Scientists. This study revealed that 82 percent of the representative sample of NBS scientists use physical properties data; 78 percent prefer data of high precision. All scientists consult with colleagues when data are required. 93 percent prefer to have the data on their own bookshelves rather than have the information centralized in the library. 73 percent expressed the need to verify or reproduce data found in the literature, and 41 percent feel it often less time-consuming to reproduce the data in the laboratory than search for them in the literature.

DR. BRADY: Are there questions?

DR. ROSSINI: What is meant by "negative replies" on several of the slides?

DR. WEISMAN: It means that we could not provide the answer or any referral. Sometimes, however, in our negative response, we have been able to check with the so-called experts at NBS and say there hasn't been any work done in this area.

DR. ROSSINI: That would be a positive reply.

DR. WEISMAN: I suppose that could be classed as a positive reply, but those were included in the "negatives".

DR. SCHULMAN: Were most of these inquiries substantive in nature? Were the inquirers asking for significant information?

DR. WEISMAN: Most of them were for information about the program or information on some publication they were interested in, or requests to be placed on our mailing list, and whether they could come to us. Some asked us for specific or substantial bodies of data.

DR. SCHULMAN: Were they mainly domestic?

DR. WEISMAN: We have had information from practically every state in this country, and from about 28 other countries.

DR. BRADY: Are there other questions?

Question: We have heard a lot about funding and lack of funding in the overall program. Do you have an ideal program in mind that you would like to see executed? What is the cost of that kind of program in relation to what you actually do have?

DR. BRADY: I had planned to take up that question in my closing remarks.

Question: What was the distribution of requests for information from government, industry, and universities?

DR. WEISMAN: The questions are from, I would say, about 30 percent from government, about 30 percent from universities and about 30 percent from private sources. We had a few from individuals whom we can't identify.

Question: In relation to the inquiries, did most of them come directly to the Office of Standard Reference Data or did they go to other offices?

DR. WEISMAN: Most of them are directed to the Office of Standard Reference Data. We do get inquiries which the offices within the Bureau, and the Technical Information Office receive, and they send them to us if they think we might be able to provide answers. Sometimes I may get in touch with a data center operator like yourself, as I have in the past, and say "We have received this query; can you reply to it?"

DR. BRADY: I think we should proceed.

Our next speaker this afternoon is Dr. Lee Kieffer who, as you can see from the program, is in charge of the Center at the Joint Institute for Laboratory Astrophysics (JILA) on atomic collision processes. He is a physicist specializing in this field and the critical reviews already put out by his center are having a profound influence on the entire practice of experimental measurements in this field, or at least they should. Dr. Lee Kieffer.

THE INFORMATION ANALYSIS;
and
THE CREATION OF RELIABLE DATA

by

Dr. Lee J. Kieffer, Director

Joint Institute for Laboratory Astrophysics Data Center

DR. KIEFFER: Since I am not responsible for the title for my remarks listed in the program I'll take the liberty of changing it. The title should read, "The Information Analysis Center and the Creation of Reliable Data". I am not going to spend a lot of time discussing the details of just what we do in the JILA Information Center. What I am going to discuss is my philosophy of operating an Information Analysis Center and what I regard as the role of such a center in the creation of scientific knowledge. Quantitative property data being one part of our scientific knowledge.

In the past, and this audience of course recognizes this as a great simplification, there were basically two kinds of Information Centers. The first was the scientific abstracting service which usually covered the formally published literature of a scientific discipline. It dealt in the raw information of science and still does. The second type was usually the lone scholar who with a small amount of clerical help sifted through the literature, consulted colleagues and then prepared a critical data compilation which he occasionally updated.

In the recent past a new and I think potentially radically different organization has entered the field. It seems now that there is general agreement it should be called an Information Analysis Center. The centers operated by the A.E.C. in the area of nuclear science are good examples. Its principal product (for the physical sciences) is critically evaluated property data. In addition it produces many products, some of which would usually be throught of as products of a scientific library function.

How can this organization be distinguished from the lone scholar. In a presentation before Dr. Ambler of NBS, I used the phrase <u>organized scholarship</u>. His almost instantaneous reaction was "that is redundant." That certainly is true. Probably a better phrase would be <u>directed scholarship</u>. I think this is not a trivial difference. It should be a group of scientifically trained scholars working together. In addition to having a potential lifetime greater than that of the lone scholar there is the critical mass effect. Another aspect of such an organization is its close connection with research groups in the area of interest. In fact the ideal situation seems to be this organized and directed group of scholars embedded in an active research group.

What I have discussed so far is I think rather noncontroversial and is what I like to refer to as "conventional wisdom". Much of what follows are personal opinions but they are tempered by discussions with many people including especially my colleagues at JILA.

When I first became involved in the information analysis business I of course floundered about for a while but when I finally felt I had my feet on the ground and knew what I should be doing, I ventured out to meet my new colleagues. For a while I was sure there must be a semantics problem. We appeared to attach different meaning to the same words. Sometime later I concluded that there was also a very basic problem. The majority of the people trying to critically evaluate property data did not recognize the paramount importance of systematic errors in assessing the reliability of the data. Their typical reaction to my needling on this point was well yes but there's nothing can be done about that. A critical evaluation of data which does not primarily concern itself with the systematic errors inherent in the measurement techniques will not in the long run be productive. Far too much of what passes for critical evaluation consists in applying superficial criteria, e.g. does the author quote the right references, is his presentation clear, does he use the correct formulas when reporting statistical errors, etc. A list such as this approximately 2 pages long was seriously proposed at a Gordon Research Conference, "Numerical Data of Science and Technology; It's Compilation and Critical Evaluation," held in 1966, as the authors' criteria for obtaining reliable data. It was a beautiful list of the criteria for the style of a first rate scientific article but it had precious little to do with the reliability of the data reported. Please don't misunderstand me. Having had to read several thousand scientific articles in the last few years, any improvement in presentation would be a godsend to those of us who actually have to read them. The most difficult part of it all is that the authors never really tell you in simple clear English, or whatever language they write in, just what they have done. They make up a story, to go along with the reported measurement, in order to convince the editor the article contains some new physics (or whatever science). So they lavish all their literary talent on the story and hardly discuss the measurement which probably is the significant thing they've done. Where does this leave us. I have concluded that it is almost impossible to evaluate the reliability of property data (or any other kind, I imagine) from what is reported in the scientific literature.

We have found in our own operation, for example, that usually some very important information necessary to evaluate the measurement is missing from the formal record which is published. This almost certainly guarantees that a repeat measurement will be necessary in order to obtain a reliable value.

Before I proceed let me make just a few general comments about the role of random errors. As we know there are some rather elegant mathematical theories to handle the random fluctuations that plague every measurement. These ideas are I think particularly useful in noting when systematic errors are occurring. They give you some real feeling for what to expect as a reasonable deviation from a previous measurement. On the other hand our real enemy is the systematic error. My own experience and that I think of every scientist who has seriously considered it is that statistical error bars are never significant in determining the reliability of the measurement.

This point was rather well put a few years ago in a paper by W.J. Youden, at the time a consultant to NBS, entitled "Systematic Errors in Physical Constants" published in Physics Today. "When two laboratories make independent determinations, each may attach to its 'best' value a ± sign followed by an estimate S of the error. This estimate of the error is often based upon a series of observations made under carefully controlled conditions. Experimenters soon discovered that if laboratories A and B reported values C_A and C_B for the same constant, the difference Δ between C_A and C_B was almost always a large multiple of their estimated error. Obviously these calculated errors had no more to do with the real errors than the neatness of the laboratory or the promptness with which the investigator answered his mail."

Determining the reliability of a measurement is not a simple problem, as anyone who has tried to do a fundamental constant measurement knows. But it is clear we have made progress in making measurements more reliably, but it is not easy. The kind of effort lavished on fundamental standards and constant measurements is the kind of effort necessary to achieve reliability in the measurement of physical properties.

Let me now define more precisely what I mean by some of the terms I have been using. Every experiment which purports to measure quantitatively a property of a well-defined physical system has a theory. This theory usually consists of a number of mathematical expressions which tell you how to connect the dial readings of the instruments to the value attached to the property. For completeness include in this scheme whatever theory is necessary to connect the instrument with the fundamental standards or secondary standards. In addition there are a number of stated or unstated assumptions about effects which in principle affect the measured value but are assumed to be negligible. [Definition] A reliable experiment is one for which all known sources of systematic error have been delimited and their magnitudes properly assessed. This includes effects noted in the formal theory for the experiment and in the stated or unstated assumptions. Data resulting from such an experiment I call reliable data. This is the best that can be done. It is of course a provisional judgment which can be overturned. If on the other hand the above statement is not true, then the theory for the experiment is defective and the data with its associated error bars are a guess.

I recently received a letter from a university professor inquiring about some ionization cross section data. He noted there were several numbers in the literature for a certain cross section and wondered what my opinion was. I reviewed the measurements and noted that <u>all</u> the techniques used in making these measurements were defective and that therefore any opinion on them was a guess and his guess was as good as mine. I think that reply epitomizes my attitude toward data coming from defective experiments.

The vast majority of data compilations in the past suffered from the fact that they were attempts to critically evaluate data from defective experiments and that therefore they relied on superficial criteria for evaluation. I really think that no one should be shocked by the notion that there are many properties we cannot measure reliably and that we are guessing.

What I have just said implies that there is probably available very little reliable property data. This is certainly true in my own field of atomic collisions and probably true outside it although in this case I am guessing, if you'll forgive me.

The criticism I have leveled at past attempts to provide reliable data do not mean that these efforts were not useful for furthering science and technology. On the contrary they were extremely useful.

But our measurement techniques (and our knowledge of what constitutes a valid measurement) are advancing at such a rapid rate that our concept of how to compile, evaluate and disseminate reliable data must change. In fact for the first time we must create a system which will be a source for archival data. Archival data is data for which enough published evidence exists for the user to determine whether a new measurement can be made which will improve the accuracy of the data and if not what is the accuracy based on the clearly stated theory of the experiment.

Science and technology have in the past taken a rather relaxed attitude toward this problem. They have counted on the fact that as knowledge and consequently measurement techniques have advanced, new, better measurements can easily be made and a lot of effort should not be expended on learning what is wrong with poor techniques. This mistake I think is now beginning to haunt us.

Techniques which were abandoned for about 35 years were recently updated using modern equipment by two different laboratories. Several years of effort were expended in each laboratory with large staffs of Ph. D.'s. Ionization cross sections were measured for electron impact on atomic helium. The results differed by about 25% and of course their quoted errors were almost a factor of ten smaller. The knowledge of defects of measurement techniques have in general been passed down from teacher to student and not documented. I think the folly of this is well illustrated by the example I just gave. I have attended numerous meetings in recent years where the validity of some theory either in the basic sciences or applied sciences turned on the reliability of some basic property data. In applied fields tremendous improvement in the reliability of complicated systems could be made if reliable property data were available to test their models.

Where can the Information Analysis Center make a contribution to this problem. First by the use of its own staff and expert consultants it must publish critical discussions of measurement techniques in order to make clear to the scientists and others making measurements which techniques are defective. Second, it must establish and publish objective criteria for judging data so that a consenus can be arrived at regarding these criteria. And finally it must publish compilations of reliable data based on the consensus about the reliability of the measurement techniques.

In the past most data compilations lacked a documented consensus about the reliability of the measurement techniques. The absolutely necessary connection between the reliability of the measurement techniques and the reliability of the data obtained must be generally recognized. In addition a consensus about the reliability of the measurement techniques must be arrived at before an archival data compilation can be produced.

In implementing the kind of program I have outlined for an Information Analysis Center the attitude of scientists poses a real problem. Scientific scholarship of the highest order is required for this work but physical scientists do not regard scholarship as an acceptable career. This is reflected in the small number of scholarly publications in the physical sciences. In the area of critical evaluation of measurement techniques the number is almost zero. We need a publication medium whose quality makes it acceptable to the scientific community so that they will contribute to it and most of all participate in reaching the consensus necessary for its success.

DR. BRADY: It is quite clear that Lee Kieffer has very definite views about the quality of data and high standards. Are there questions?

DR. SCHULMAN: All of us want accurate information, whether it is in special publications or in regular journals, so what can be done?

DR. KIEFFER: We just need publication media of some sort which societies will be interested in getting behind, in which sufficient detail can be expressed. We need something new!

The real problem is that a few years most physical ideas were based on rather qualitative experiments. You either saw the line or you didn't! At that time this kind of attitude was quite acceptable. The point was proved and a new idea in physics was born. But today in studying complicated physical systems, if you really want to find out how reliable a model is for the atmosphere, or whatever, you need numbers that are reliable. If you don't have reliable numbers you are in trouble.

DR. BRADY: Dr. Garvin has a question.

DR. GARVIN: I think your remarks about scientists and scholars are very well taken and what you say about the need for a new method of publication I also feel is true. The problem simply is this: The present journal policies are based on economics. An extended evaluation or a discussion of criteria based on reworking of available data is expensive. This is viewed as secondary processing of physical data.

There are no good outlets for what I will call an independent evaluator to present the results of re-analysis of data. When I say an "independent evaluator" I am excluding those who work for an organization devoted to putting out evaluations. The man who is an expert in a small area, who is interested in this kind of work, has no independent outlet where he can put out an evaluation. This being the case, we are losing the part-time services of a very large part of the scientific community, namely, the people who are doing experiments or analyses on small systems the result of which would be of interest if they could be presented. It is not clear what is needed. Perhaps results or special sections in the present journals.

DR. MARVIN: Concerning the question of how you can get the journals to recognize this problem, I think a responsibility rests with all of us when we are asked to serve as referees of papers. We all know that the problem of evaluating a paper is a very difficult one. As a matter of fact, it boils down to a small job of critical evaluation and most of us hate spending the amount of time necessary to do this.

It has been my experience that when we do spend the necessary time to do a really good job of refereeing - and it may be a couple of weeks sometimes - the editors generally are very grateful for it and will pay attention. I think if all of us could persuade ourselves, and our colleagues also, to really make an effort to be very critical, very strict in our evaluations of the papers we are called upon to referee and point out where papers are lacking in the information needed to evaluate them, we would find an enormous improvement in the literature. There is no question about it: It is a lot of work.

DR: BRADY: One more comment and then we will turn the meeting back to Dr. Rossini.

MR. HILSENRATH: I think we got away from a point that Dr. Kieffer made. I think we ought to be generous and say that when we pick up papers today, we find that the author has put all the wrong information in the paper. The things we really want to know about are not there.

The next question would be: Does the author really know what to put in the paper? That is something I don't think the journal can help on. What are we going to do about getting the message to people on the pertinent information to put in a paper describing the experiment?

DR. BRADY: Dr. Rossini has a final remark on this subject.

DR. ROSSINI: I just wanted to call attention to the fact that this is a real problem which Dr. Kieffer has pointed out. However, it is different in what you might call the highly developed areas of science from what I would call the underdeveloped or the new areas. For example, in the area of themodynamics which I would call rather highly developed, Dr. Waddington referred to a Resolution that the Calorimetry Conference published which spelled out very clearly what the investigator should put in his paper. It may well be then that for the other areas, we have to begin promoting this sort of thing. Thank you, Ed.

SUMMARY

By

Dr. Edward L. Brady

DR. BRADY: I would like to close this session with a few remarks. Most of us from the Office of Standard Reference Data, as you have noticed, have made remarks about the scarcity of financial resources. The question has been asked "How much money do we actually have? What is the magnitude of the program?" For Fiscal Year 1968, the National Bureau of Standards had $1.86 million for the program. As a result of the legislation that was passed by Congress, the authorization that we received for FY 1969, the current year, was exactly the same figure, $1.86 million. If it hadn't been for this very welcome legislation, we might have had more money for this year. But hopefully, in the future, the legislation will give a basis for expanding considerably.

Now, this $1.86 million is only the NBS portion. We have also talked about activities under the sponsorship of the AEC, the DOD, NASA, and so on. These other agencies taken altogether, according to our estimate, invest another $3-1/2 million or so in data compilation, so the total is of the order of $5 million to $5-1/2 million total investment in these activities throughout the major technical agencies of the Government. We estimate that this figure is between one-fourth and one-third the level necessary to cover the main areas of science at a reasonable level such that we can, within a period of a few years, hope to become reasonably current.

Finally, what sort of interaction are we hoping to get from the members of the Advisory Board of the Office of Critical Tables? Why did we ask you to come here today to listen to our story. We don't want this story to be a monologue at all. We look for a dialogue between us in the Office of Standard Reference Data and the members of the technical community, directly with us and through the medium of the Office of Critical Tables, through the medium of professional societies, and any other useful channels that can work. Most of the members of the Advisory Board are representatives of organizations. They are named to this committee because they do represent important organizations. We ask you to be channels of communication with your organizations to initiate discussions between the members and us about their needs and we particularly want to know what we might do that can be helpful to you and the directions that we ought to take in the future.

We thank all of you, the members of the Advisory Board, and other participants for coming here today to listen to our reports. We look forward to many years of service to the technical community producing critical reviews, data compilations, analyses of the sources of error in experiments and all of the other kinds of benefits that critical evaluation of the numerical data in the literature, and other sources, can produce for us. Thank you very much.

I now return the program to Professor Rossini.

CLOSING REMARKS

By

Dr. Frederick D. Rossini

In the program today, we have been given a summary of the situation in the United States and somewhat throughout the world on the problem of critical tables of reference data for science and technology.

While a great deal has been accomplished in the United States in the eleven years since the establishment of the Office of Critical Tables, and in the five years since the setting up of the National Standard Reference Data Program at the National Bureau of Standards, very much remains to be done.

In addition to proceeding expeditiously on our program in the United States, bringing together the governmental, industrial and university capabilities and resources, we must work to keep the international program going forward in a way that will truly benefit the scientists and technologists in the world.

I urge the Members of Our Advisory Board, and our guests, to send in whatever comments they may have about the reports presented here today, about the program of the Office of Critical Tables to Dr. Guy Waddington, and about the National Standard Reference Data Program to Dr. Brady.

Also, I am sure that the Members of the Executive Committee of the Office of Critical Tables would appreciate receiving comments and suggestions. They are:

Dr. Robert Brode, of the University of California at Berkeley, representing the NRC Division of Physical Sciences,

Dr. Sydney Clark, of Yale University, representing the NRC Division of Earth Sciences,

Dr. John Margrave, of Rice University, representing the NRC Division of Chemistry and Chemical Technology,

Dr. George Holbrook, of the du Pont Company, and Dr. John Cottman, of the Westinghouse Company, both representing the NRC Division of Engineering, and

Dr. Allen Astin, Director of the National Bureau of Standards, who is a Member Ex-Officio.

In bringing this meeting to a close, I want to express our sincere thanks and appreciation to all the speakers, to all the Members of the Advisory Board, and to our Guests, for their participation in today's program.

I also extend our sincere thanks and appreciation to Dr. Waddington and his staff for their good work in handling all of the arrangements for this meeting so efficiently.

Dr. Waddington has informed me that the proceedings of this meeting will be prepared and subsequently distributed to all participants.

We hope that the reports and discussions of our meeting today have been helpful to all participants.

We look forward to working together in a mutually beneficial way in both the private and the government sectors of our scientific-technical community in a cooperative program leading to the provision of adequate numerical data for science and technology in the United States.

The meeting is adjourned.

THE METALS PROPERTIES COUNCIL

What The Metal Properties Council Has Done and Is Doing

I - For materials for boilers and pressure vessels.

1) Assembled data on carbon and alloy steels by mail solicitation. Pooled this with material on hand with the A.S.M.E. Boiler and Pressure Vessel Code Committee.
2) Now analyzing and arranging this material for publication, scheduled for October, 1968.
3) Analyzing accumulated data of the Boiler and Pressure Vessel Code Committee and the Joint Committee to make it available to engineers in useable form. First of probably six volumes now in process of publication.
4) Conducting a review (using computer equipment) to see how well this accumulated data supports standard parametric methods of projection. Results will be published this Fall.
5) Instituted a two year program to develop a method of parametric evaluation superior to those now in use.
6) Started a testing program of certain aluminum alloys, results to be published in about a year. This program includes creep and stress rupture data using the most recent techniques.
7) Sponsored a symposium at an ASME-AWS Annual Meeting on the Properties of Weld Deposited Metal at Elevated Temperatures. This has been published by ASME.
8) Sponsoring with the Joint Committee a symposium on Creep and Creep Testing to be held October 14th at the Metals Congress.
9) Planning new data solicitation on certain alloy steels presently widely used in pressure vessel construction.

II - For increasing our knowledge on how to utilize quenched and tempered steels particularly at elevated temperatures, in welded construction, and in hostile environment.

1) Sponsored a symposium at an A.S.M.E. Petroleum Division Meeting which was published by that organization.

2) Conducted an analysis of the papers at the symposium, together with bibliography, and published this through A.S.M.E.
3) Initiated a long time elevated temperature testing program on 4-1/2 inch thick quenched and tempered chrome molybdenum steel plate. This program will yield data on embrittlement as well as on creep and stress rupture. First results should appear in about two years.
4) Planning extension of the program to other alloys.

III - For obtaining data on low cycle fatigue characteristics of metals:

a) As applied to central station power generation equipment and petroleum refining and chemical processing equipment.
b) New data on fatigue characteristics of certain aluminum alloys.

1) Obtained a chrome moly vanadium steel turbine rotor forging, and some chrome molybdenum steel large diameter heavy walled pipe. Started a program of thoroughly testing this material for identification, preparatory to a program of precisely cycled fatigue testing. The fatigue testing program will begin in December.
2) Started a testing program of certain aluminum alloys using new sophisticated equipment and techniques.

IV - For studying the effects of the rate of loading on the strength of metals.

1) Instituted a cooperative program with three company laboratories which are testing three metals at various temperatures and rates of loading to establish guideposts for a larger program.
2) Planning a symposium on this subject in 1969.
3) Conducted a search in existing data banks and assembled an extensive bibliography on the subject. Studied all data bank references and prepared an interpretive report on the subject which is now in process of publication.

4) Intends to use the interpretive report and the cooperative program as a basis for a larger scale program starting in 1969.
5) Initiated a testing program of aluminum alloys at extremely high rates of loading.
6) Planning a testing program of aluminum alloys at low rates of loading.

V - To determine the relaxation characteristics of metals.

1) Search in existing data banks, plus a mail solicitation has brought forth a large amount of data plus previously unpublished reports which are now being analyzed first for publication; and, second, for setting up whatever program might be needed. Program to begin in 1969.
2) An interpretive report is now in preparation for publication this Fall.
3) Studies are being made for the optimum presentation of data, preparatory to completely revising the current work on this subject. (A.S.T.M.)
4) A symposium and a workshop session on this subject are planned for 1968 and 1969.
5) A testing program on relaxation characteristics of aluminum alloys has been started which will be completed in about a year.

VI - To analyze the effectiveness of surveillance test programs to determine the effects of irradiation on the properties of metals.

1) Formed a Task Group and a Subcommittee to guide MPC activities in this area.
2) Has assumed responsibility of gathering and analyzing surveillance test data from power installations.
3) A publication is in preparation on this subject. This will be the first published analysis of actual surveillance test data.

VII - To determine the properties of aluminum and titanium in large sections.

1) A Task Group has gathered data on this subject from manufacturers. It is being analyzed by Air Force facilities for inclusion in their Manual, following which it will be arranged and published.
2) Further plans are being made to supplement existing data.

VIII - In the field of Fracture Characteristics:

1) Organized a Task Group which is determining the role MPC is to play in this area.
2) Set up two test programs for aluminum alloys, which are under consideration for early implementation.

IX - In the field of Corrosion:

1) Organized a Task Group which is considering what MPC might do regarding corrosion characteristics of metals.

X - With regard to the Joint Committee:

1) MPC now raises funds for the ASTM-ASME-Joint Committee on the Effects of Temperature on the Properties of Metals.
2) This Committee has just published a work on superalloys.
3) Planning a number of symposia in 1969, as well as two important research programs.
4) Has just started a unique program to obtain actual data on the relation of notch effect to the size of specimens.

List of Mechanical Properties

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. <u>Non-Crystalline Substances</u>

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. (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.

The Preparation of Critical Reviews for Selected Areas of Chemical Kinetics

The Problems

Perhaps the most important difficulty in attempting to provide satisfactory coverage of the chemical kinetic literature is the number of variables which must be specified in the description of a single experiment. The influence of solvents, diluents, in gas reactions, "inerts" present for purely practical reasons, pressure, volume and temperature ranges or values, composition variables plus the bewildering variety of catalysts is not sufficiently understood to permit categorical rules for the further presentation of data. Further, the sensitivity of reaction rate to temperature makes it impossible for the experimenter to carry out his measurements at an arbitrary temperature which is convenient for the data compiler: extrapolation of data always introduces the possibility of a change in mechanism and of entirely meaningless kinetic parameters.

The question then is as to the best method of representing the state of chemical kinetic experimental data today in a critical way. For one concerned with compiling data from the literature there are a number of alternatives:

The actual experimental data content of the published paper

This is an unbiased statement of an experimental contribution provided in reduced format (such as a fitting function) with error bounds on the actual data. The principal difficulty here is that the article generally does not provide unprocessed data in full -- generally only an illustrative example. Full information might be available from the experimenter if a cooperative program could be worked out.

Data content together with proposed mechanisms

Since kinetic experiments are often initiated with the goal of deciding between differing theoretical reaction mechanisms, perhaps the path of the reaction suggested by the experimenter should also be included, particularly so as to permit critical review at some time of the corpus of data in a specific area. This is material which is extremely difficult to tabulate; the result tends to resemble isolated paragraphs from a monograph rather than a useful table.

Derived kinetic parameters

This is the approach taken so far. Data immediately available from the vast majority of journal articles has been processed on the basis of a reaction mechanism and reduced to standard kinetic parameters. It is essentially impossible to recover the original information content of the experiment or its precision if alternative theories of reaction path should be proposed, hence the experimental work must generally be repeated to establish the theory.

A second question relates to the problem of evaluation. Should this be a matter of experimental precision? On the basis of soundness and widespread acceptance of mechanism and the agreement of experimental data with it? Or a combination of both as establishing a standard chemical kinetic parameter for a specific reaction? The difficulties inherent in establishing one numeric as a critical value in chemical kinetics are enormous, as compared with, e. g., thermodynamics.

A Possible Solution

A survey of compilations and review publications in this field indicates that first, they are not timely -- the cut-off date on bibliographic research is sufficiently in the past that the reader cannot be at all sure that the material may not be completely out-dated; and second, they are generally encyclopaedic. The tendency is to cover all reports of any experimental material relating to reaction rate studies published during a particular period and must, therefore, present only a guide to the literature, not a set of useful, factual items of information directly applicable to the solution of the readers' problem.

One possible way out of the dilemma is proposed here as a two-part program. In the first place it is acknowledged that with all of the uncertainties as to its ultimate usefulness, the process of abstracting and codifying the literature of chemical kinetics must be continued in some fashion, or the sheer bulk of the backlog of published information will cause a major fraction of it to disappear forever. Therefore, an immediate program of continuing the activities previously in course of reducing the published information on chemical kinetics to a compact form will be instigated. Present thinking tends toward a preference for some form of empirical representation of raw data whenever this can be done, perhaps with some form of indication as to the mechanism proposed. This is essentially a rear guard action, not in itself designed to be of any immediate help to research workers in kinetics, but as a buttress to the second phase of the program.

The primary action needed is considered to be that of critical review, in depth, of a large number of narrow areas of chemical kinetics. These reviews are envisaged as being carried out by acknowledged experts in the areas, treating a very specific subject, using whatever bibliographic assistance the continuing data file program can provide and producing in a relatively short time a definitive and up-to-date monograph on the state of the art and the standard reference data when available in the area under consideration.

This requires reviewers who are competent in the various subdivisions of chemical kinetics -- particularly in the eyes of their peers -- who are willing to undertake the task, dropping a part of their own research, and spending six to twelve months (our present estimate) in this type of activity. It also requires that the field of chemical kinetics be fragmented into units which can be reviewed thoroughly in such a period of time. Finally, it requires that the product of this effort must be produced in an acceptable form for the use of the scientific public.

Neither a logical nor an arbitrary subdivision of chemical kinetics will assure that a competent reviewer, willing to do the work, will exist. The only reasonable course would seem to be to first choose the reviewers: this choice will automatically fragment the field into subdivisions which can be satisfactorily updated and standardized. Further, it should make much clearer the areas in which this kind of critical review are needed, and the kind of person best suited to do the work. Finally, it should become quite clear which aspects of kinetics are absolutely blank, as regards quantitative data and acceptable reviewers, and lead perhaps to useful activity in their investigation.

The Critical Chemical Kinetics Monograph

The reputation and acceptance of such monographs will depend on four points. First, the selection of authors in the several fields who are adjudged by others in the same and overlapping areas to be the best authorities on the subject; second, the care, thoroughness and depth of the investigation, and the timeliness of the finished publication; third, the prompt production in a pleasing format of the publication and its efficient distribution; fourth, the development of a basic set of rules for the organization of information in the monographs with regard to information on theory and experiment -- including critiques of methods -- and a rigid adherence to these rules so as to provide coherence in the series.

In any of these fragmented areas of chemical kinetics this publication should supersede any other monographic work. Research workers, whether new graduate students or seasoned research men considering a new field of specialization, need to explore the literature only after the date of writing. This endeavor is not intended as simply a proliferation of printed pages.

Production

In order to produce such a series of monographs, ultimately spanning the whole field of chemical kinetics and defining the standard, best current values of kinetic parameters, these steps are proposed:

Preparation of a listing of perhaps fifty reviewers, each a specialist in some particular area of kinetics. This number is a preliminary estimate based on a presumed cost of about $5, 000 per contractual agreement and subject to the availability of the necessary funds.

Contracts will be let for the preparation of manuscripts in a time period to be agreed upon according to standard procedures. Graduate student and other second level assistance will presumably be a part of the task force but responsibility for the quality and timely completion of the project will rest with the senior author.

Upon receipt of the manuscript, and its certification by the National Bureau of Standards as satisfactory, the monograph will be produced for public distribution as rapidly and inexpensively as is consistent with accuracy and good taste and made available through the usual channels to the scientific community .

Organization of the Monographs

A preliminary plan of the organization of the monographs includes the following major points:

They should include a comprehensive bibliography to a cut-off date of all significant activity in the area. Where omissions are made it should be clear from the text why this is reasonable.

Where the state of the art warrants it, kinetic parameters which can be considered "standard" should be collected and displayed. The implication here is that there is general acceptance among workers in the field as to theory and mechanism, as well as a definite decision among several sets of data as to the precision of the data chosen.

When there is no clear agreement as to the mechanism, but experimental data is available, wherever possible the unreduced, "raw" data should be critically examined the best representation of the body of such data determined and presented, together with standard statistical estimates of its precision. Thus, where theory is in doubt, later workers should not have to search the literature for numerical data to compare with new theories or new experimental work.

Finally, in the case where neither a satisfactory theoretical basis or an acceptable body of experimental data (except in the sense of purely qualitative indications) are to be had, this situation should be positively stated. Perhaps the latter of these should be displayed in the best cases. Areas such as these in which experimental research is needed must be identified just as much as the critical numerical values need to be delineated in other fields which have been worked over for many years.

<u>In summary:</u> A critical chemical kinetics monograph must be a complete, rigorous and definitive summing up of the particular area of chemical kinetics chosen. It should permit a non-expert in the field -- as mentioned before, whether a novice just beginning research or a professional research man seeking out an area of interest -- to read this publication and know, as of the date of publication, essentially the exact state of scientific knowledge, both theoretical and experimental in such combinations as circumstances dictate.

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(The Mineralogical Society of America)
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(The Geochemical Society and Society of Economic Geologists)
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(National Aeronautics and Space Administration)
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J. L. Margrave, Rice University, Houston, Texas (was unable to attend)

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National Bureau of Standards, Office of Standard Reference Data

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Carla Messina, National Bureau of Standards, Washington, D. C.
John Sanderson, Optical Society of America, Washington, D. C.
B. L. Shapiro, Texas A & M University, College Station, Texas
F. Y. Speight, Engineers Joint Council, New York, N. Y.
R. C. Thompson, National Bureau of Standards, Washington, D. C.
J. I. Vette, Goddard Space Flight Center, Greenbelt, Maryland
J. B. Wachtman, Jr., National Bureau of Standards, Washington, D. C.
Mary Warga, Optical Society of America, Washington, D. C.
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Eloise Batchelor, Office of Critical Tables
J. W. Berg, Jr., Division of Earth sciences (unable to attend)
Barbara James, Office of Critical Tables
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M. A. Paul, Division of Chemistry and Chemical Technology
N. E. Promisel, Materials Advisory Board
G. C. Sponsler, Division of Engineering (unable to attend)
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