

Directory of Continuing Numerical Data Projects: A Survey and Analysis (1961)

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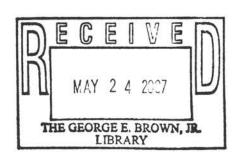
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DIRECTORY OF Continuing Numerical Data Projects

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by the Office of Critical Tables
1961



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FOREWORD

This is the first issue of a directory of projects that compile and publish the numerical data of science and technology on a continuing basis. It was prepared in the Office of Critical Tables of the National Academy of Sciences-National Research Council. Revisions will be published at more or less regular intervals. The original purpose of the directory was to aid the Office in the coordination of existing data projects and the stimulation of new ones. It soon became apparent, however, that the directory would be of use to others. Accordingly the Advisory Board and Executive Committee of the Office have concurred in its publication in the present form.

The directory covers the activities of more than 30 data compilation groups located in the United States and Europe. The projects have been grouped, according to the properties they cover, into physicochemical, crystallographic and mineralogical, nuclear physics, thermophysical, spectroscopic, and comprehensive projects.

The directory was prepared by M. Joan Callanan under the supervision of Guy Waddington, Director of the Office of Critical Tables. Thanks are due to Members of the Advisory Board of the Office of Critical Tables, project directors, and others for information and suggestions.

> A. V. Astin Chairman, Executive Committee Office of Critical Tables

Z7405.T3 D54 1961 c.1 Directory of continuing numerical data projects: a survey and analysis /

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THE OFFICE OF CRITICAL TABLES

The Office of Critical Tables operates jointly under the following Divisions of the National Academy of Sciences-National Research Council: Chemistry and Chemical Technology, Earth Sciences, Engineering and Industrial Research, and Physical Sciences. The five-man Executive Committee of the Office consists of a chairman and representatives of the four Divisions. The Committee works closely with the staff. It is responsible for over-all policy and program, and provides expert guidance on major aspects of the operation. Its present membership is:

Chairman:

Allen V. Astin, Director, National Bureau of Standards

Chemistry and Chemical Technology:

Frederick D. Rossini, Dean, College of Science, University of Notre Dame

Earth Sciences:

Francis Birch, Professor of Geology, Harvard University

Engineering and Industrial Research:

J. R. Townsend, (Ret.) Bell Telephone Laboratories, Inc.; Consultant to Director of Defense Research and Engineering, Department of Defense

Physical Sciences:

Robert B. Brode, Professor of Physics, University of California at Berkeley

The Office staff develops and carries out the general program outlined by the Executive Committee. As of December 1960 the staff included the following professional members: Guy Waddington, Director; Richard Wiebe, Assistant Director; M. Joan Callanan; Senta Raizen; and Carol Schiller. The Office is currently supported by a National Science Foundation grant.

The Advisory Board of the Office, which is a source of expert knowledge in the many areas of compilation activities, consists of seventy-off members. It is comprised of representatives of prominent scientific, engineering, and technological organizations in the United States; representatives of government agencies; and a number of members-at-large having special interest or competence in the compilation of critical data. The organizations and agencies currently represented are:

A. PROFESSIONAL SOCIETIES

Acoustical Society of America American Association for the Advancement of Science American Astronomical Society American Ceramic Society American Chemical Society American Crystallographic Association American Documentation Institute American Geological Institute American Geophysical Union American Institute of Chemical Engineers American Institute of Electrical Engineers American Institute of Mining, Metallurgical, and Petroleum Engineers American Institute of Physics American Meteorological Society American Oil Chemists' Society American Physical Society American Society of Biological Chemists American Society of Civil Engineers American Society for Engineering Education American Society of Heating, Refrigerating, and Air Conditioning Engineers American Society of Mechanical Engineers American Society for Metals American Society for Testing Materials Electrochemical Society, Inc. The Geochemical Society Geological Society of America Illuminating Engineering Society Institute of the Aeronautical Sciences Institute of Radio Engineers

Mineralogical Society of America Optical Society of America Seismological Society of America Society of Automotive Engineers Society of Economic Geologists Society of Naval Architects & Marine Engineers Special Libraries Association

B. INDUSTRIAL ASSOCIATIONS

Aircraft Industries Association of America American Iron and Steel Institute American Petroleum Institute Industrial Research Institute Manufacturing Chemists Association Textile Research Institute

C. UNITED STATES GOVERNMENT

Agricultural Research Service, Department of Agriculture Air Force Office of Scientific Research Army Office of Ordnance Research Bureau of Mines, Department of the Interior Bureau of Reclamation, Department of the Interior Coast and Geodetic Survey, Department of Commerce Geological Survey. Department of the Interior Los Alamos Scientific Laboratory, Atomic **Energy Commission** National Aeronautics and Space Administration National Institutes of Health Naval Ordnance Laboratory Naval Research Laboratory Office of Naval Research Smithsonian Institution Weather Bureau, Department of Commerce Wright Air Development Division, Dayton, Ohio

INTRODUCTION

Thirty years have passed since the publication of the last volume of the INTERNATIONAL CRITICAL TABLES OF NUMERICAL DATA. The ICT, which was prepared under the auspices of the National Academy of Sciences-National Research Council, continues to serve science and technology even today. Since its publication, however, there has been a tremendous increase in the amount of numerical information of value to research. A number of independent groups are making efforts to consolidate and evaluate the data of selected areas of science, but the task is far from complete and lacks coordination. To cope with the situation the Academy-Research Council in 1955 authorized formation of the Office of Critical Tables. The Office became operative in late 1957. 2

The program of the Office includes the following related aims: to survey the needs for critical tables of numerical data, to stimulate and coordinate the preparation of critical tables, to develop standards for the presentation of numerical data, and to provide a central index of critical numerical data. The identification of all continuing projects now in operation that compile and publish numerical data and an analysis of the quality of data being compiled by these projects are necessary first steps in the achievement of these aims.

Accordingly information on the organization and administration, scientific qualities, and publication procedures of more than 30 data compilation groups has been collected. A condensation of this information is presented here in the form of a directory. The file on existing projects will be kept current; the search for new projects will continue, and revisions of the directory will be issued at appropriate intervals.

Admittedly the selection of activities to include in the directory has been somewhat arbitrary. Activities such as the American Petroleum Institute Research Project 44 - which have a well organized and productive program for the collection, selection, publication, and revision of numerical data - qualify without question as "continuing projects." Decisions about less formal activities have been more difficult to make.

McGraw-Hill Book Company, Inc., New York, 1926-1930.
See pages viii-ix for a description of the organization of the Office.

For example, some "projects" have qualified as such because responsible groups or individuals have undertaken (1) the long-term compilation of numerical data in a broad area of science, or (2) the frequent revision of data books of established value. The publication of ATOMIC ENERGY LEVELS by the National Bureau of Standards is an example of (1); the revision of DANA'S SYSTEM OF MINERALOGY by Harvard University scientists - the seventh edition is now in process - is an example of (2).

It is easier to explain what have not qualified as projects. Not included in this directory are encyclopedias, such as BEILSTEIN'S HANDBUCH DER ORGANISCHEN CHEMIE, which include other than numerical data; handbooks, which cover many areas of knowledge; and data centers that provide specialized information services rather than compilations of enduring value.

Another type of compilation not included in this edition of the directory is the single or occasional publication of numerical data for which there is no systematic plan for revision and extension. Many of these publications serve as excellent sources of numerical data and will be incorporated into the over-all program of OCT. A selected list of such publications, now in preparation, will be issued either as a supplement to this edition of the directory or as part of the next edition.

The data projects that are included in this directory differ in their aims and in the procedures used to achieve their aims. Some projects publish only those property values that have been evaluated with great care; others publish data of variable quality because urgent needs preclude critical evaluation of all available information; a few compile all values and leave the choice of a value to the user. Projects might have been classified and grouped according to these differences. However, a rigid classification is difficult to make since the lines of demarcation between types are not sharp. Furthermore, new projects are particularly hard to classify since their procedures are not well established.

For presentation in the directory, projects are grouped according to the classes of properties they cover. This grouping serves two purposes: (1) It provides quick and easy reference for those who are interested in the activities in one area of science. (2) It highlights the fact that existing projects are concentrated in relatively few areas of science.

The general categories of projects in this directory are as follows: (I) Physicochemical Projects (of which the greatest number deal with chemical thermodynamic properties), (II) Crystallographic

and Mineralogical Projects, (III) Nuclear Physics Projects, (IV) Thermophysical Projects, (V) Spectroscopic Projects, and (VI) Comprehensive Projects. Spectroscopic Projects are subdivided into those that deal with atomic, infrared, electronic, and other types of sprectra.

Within each general category or subdivision, projects have been listed alphabetically by name. Only a few have official names. For the others names have been assigned that will serve to identify the activity. Very often the name assigned is that of the most important publication issued by the project.

Information about the projects is given under the following headings: organization; substances; properties; sources of data; criticality; use of nomenclature, symbols, units, physical constants; currency; format; and publication and distribution. All these headings are self-explanatory with the possible exception of the term "criticality." As used in the directory, this term refers to the critical evaluation of data. Under this heading is given an indication of the criteria and methods used by project staffs in the data evaluation process.

For many of the projects it has been possible to obtain up-to-date information from direct sources. For others, direct sources were not readily available or recent changes may not have come to our attention. It is also possible that the information obtained, directly or indirectly, has not always been correctly interpreted. For these reasons corrections or additions to the directory may be necessary. The Office of Critical Tables would therefore appreciate receiving from readers any information that will make the project descriptions more accurate and complete. The Office is also eager to learn of other activities both in the United States and abroad that may qualify as continuing numerical data projects. ² General comments on the directory - its content, arrangement, format, etc. - are also welcome. Correspondence should be addressed to the Office of Critical Tables, National Academy of Sciences-National Research Council, Washington 25, D. C.

[&]quot;Thermophysical properties" is a term coming into common use. It includes thermodynamic and transport properties involved in physical change.

Several recently established activities, brought to the attention of the Office too late for inclusion in this edition, will be included in the next.

I. PHYSICOCHEMICAL PROJECTS

I-1. American Petroleum Institute Research Project 44

Organization: This project, established in 1942 at the National Bureau of Standards in Washington, D. C., was transferred in 1950 to the Carnegie Institute of Technology in Pittsburgh, Pa. In early 1961 the project was moved to the Department of Chemistry, Agricultural and Mechanical College of Texas, College Station, Texas. The project is sponsored and financed by the American Petroleum Institute. Until 1960 it was directed by Frederick D. Rossini who was succeeded by Bruno J. Zwolinski. The staff includes about twelve full- and part-time professional workers, plus supporting editorial and office help. A six-man Advisory Committee provides guidance and liaison with industry. There has been continuous and steady effort from this project since its inception. Close contact is maintained with related experimental work.

<u>Substances</u>: Hydrocarbons and related compounds of oxygen and sulfur.

Properties: Values are given for the following physical and thermodynamic properties--cryoscropic constant; density; (dt/dp); refractive index, specific dispersion; surface tension; temperatures of boiling, melting, sublimation, and transition; vapor pressure; viscosity; molal or specific volume; activity coefficient of gases; coefficient of compressibility; critical compressibility, density, pressure, temperature, and volume; free energy, heat, entropy, and equilibrium constant of formation; heat capacity; free energy function; heat content function; free energy; heat content; entropy; heat of combustion; heat and entropy of phase changes; standard heat, standard entropy, and standard free energy of vaporization. Property values are presented at standard reference points and selected intervals of the variables (temperature. pressure, etc.) over ranges dictated by probable use of the data and reliability of the extrapolation methods. (APIRP 44 also publishes several types of spectra. See V-B-1, V-C-1, V-D-1, V-E-1, and V-F-1.)

Sources of Data: Original papers in the literature, available unpublished data, original calculations.

<u>Criticality</u>: The experienced staff carefully evaluates the available data. Reliable correlation methods are used to create data for compounds not studied and quasi-theoretical methods to extend the range of variables beyond the limits of convenient experimentation. After evaluation and correlation, "best" values are selected. The methods of data treatment create internal consistency within related bodies of information. The introduction to the publication includes a discussion of criteria used to evaluate, and methods used to create, data. From time to time, staff members publish journal articles on the general philosophy and methodology of the project and on specific techniques employed.

Use of Nomenclature, Symbols, Units, Physical Constants: New recommendations of authoritative national and international committees are adopted in ways and at times that will cause a minimum of change in the extensive tabulations.

<u>Currency</u>: Revisions and additions are issued at regular intervals. In many instances data are made available to the scientific public in less time than through regular (journal) channels.

Format: The primary publication form is the 8" x 10 1/2" loose-leaf sheet coded according to substance and property. Physical and thermodynamic data are tabulated on one side of the sheets. No complete index is given but substances are logically arranged according to the Standard Order System which is based on the periodic table. Specific references (authors' surnames only) for each entry in the data tables are tabulated on separate sheets. Complete references are found in a general list of references. Bound volumes consolidating the current values of physical and thermodynamic properties were published in 1947 and in 1953.

Publication and Distribution: The covering title of the loose-leaf sheets is SELECTED VALUES OF PROPERTIES OF HYDROCARBONS AND RELATED COMPOUNDS. As of June 30, 1960, there were 2021 valid sheets pertaining to physical and thermodynamic properties. Of these, 1517 were sheets of tables. New sheets are distributed semiannually by the Agricultural and Mechanical College of Texas, Department of Chemistry, College Station, Texas. Distribution of the sheets is made to three categories of recipients: (1) contributors to the research fund of API - complimentary copies; (2) university departments, nonprofit research institutions, government organizations, and independent free libraries - free copies, one set each; and (3) other interested persons - copies by sale. The sheets are sold, in complete sets only, at five cents per sheet. The 1947 bound volume, SELECTED VALUES OF PROPERTIES OF HYDROCARBONS, was published by the National Bureau of Standards as Circular 461 (xiii + 483 pp.) and the 1953 volume, SELECTED

VALUES OF PHYSICAL AND THERMODYNAMIC PROPERTIES OF HYDRO-CARBONS AND RELATED COMPOUNDS, by the Carnegie Press (ix + 1050 pp.). The 1953 volume is available for \$7.00 from Carnegie Press, Carnegie Institute of Technology, Pittsburgh, Pa. The physical and thermodynamic data valid as of December 31, 1957, are also issued on 51,286 IBM punch cards. These are available, in complete sets only, at one and a half cents per card from the Agricultural and Mechanical College of Texas, Department of Chemistry. A new fifth supplement of cards is in preparation to include the data valid as of December 31, 1959.

I-2. Chemical Kinetics Data Project

Organization: This project was established at Princeton University in about 1952 under the direction of the late Professor N. Thon. Charles H. Stauffer became project director in 1954 and has continued the work, first at Worcester Polytechnic Institute and since 1958 at St. Lawrence University, Canton, N. Y. Administrative supervision is provided by the Division of Chemistry and Chemical Technology of the National Research Council and technical supervision by the NRC Subcommittee on Kinetics of Chemical Reactions. The National Bureau of Standards aids the project particularly by publishing the final results. The Office of Ordnance Research provides financial support under contract with NRC. On the staff are a number of expert collaborators in various universities and chemistry department members from St. Lawrence University.

<u>Substances</u>: Inorganic and organic reactions are reported whether in the gaseous, liquid, or solid phase.

<u>Properties:</u> Values are given for the following for reactions occurring in homogeneous systems--rate constants, activation energies, frequency factors, activation heats, and activation entropies. Where no rate constant can be derived from the available data, empirical rates are sometimes given. The medium (solvent), amounts of addends (catalysts), temperatures, and concentrations are specified.

Sources of Data: Open literature.

<u>Criticality</u>: Experienced scientists carefully evaluate the available numerical data on reaction rates. Stress is laid throughout on experimentally ascertained facts. Kinetics measurements by their nature are often not very precise, but where possible values are averaged or "selected." A short presentation of additional information pertinent to the evaluation is sometimes given in a "comments" section.

Use of Nomenclature, Symbols, Units, Physical Constants: A systematic effort has been made to conform all results to a uniform mode of presentation based on time in seconds, concentration in moles per liter, and temperature in °C; rate constants are based on natural logarithms. Other usages are those generally accepted by experts in the field.

<u>Currency</u>: The staff is able to keep abreast of the literature but publication of results is infrequent. Omissions from earlier years are added to each book. There is no interim distribution of loose-leaf sheets.

Format: The publication form is a collection of 8 7/8" x 11 3/8" loose-leaf sheets assembled in book form under paper covers. The numerical data are presented entirely in tables, the patterns of columns and headings varying somewhat from one table to another, depending on their contents. Under each reaction type, reactions are arranged and numbered within the table in the order of increasing complexity of the key reactant. There is a subject index based on a classification of reactions according to type and an alphabetical index of reaction types. There is also an alphabetical index of the classes of compounds involved in the reactions published so far. Literature references used or mentioned in comments are appended to each table; references examined but neither used nor mentioned are not given.

Publication and Distribution: The volumes of this project are published as NBS Circular 510 under the covering title TABLES OF CHEMICAL KINETICS - HOMOGENEOUS REACTIONS. Circular 510 (xxiv + 731 pp.) appeared in 1951, Supplement 1 to Circular 510 (xiv + 472 pp.) in 1956, and Supplement 2 (iv + 37 pp.) in 1960. Supplement 2 is a cumulative alphabetical index of the classes of compounds covered in Circular 510 and Supplement 1. These volumes are available from the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C., for \$4.00, \$3.25, and 35 cents, respectively. NBS makes a secondary distribution to cooperating and sponsoring groups, government agencies, and other qualified domestic and foreign users of chemical kinetics data. Material for another supplement of reaction data will be ready for publication in late 1960.

I-3. Contributions to the Data on Theoretical Metallurgy

Organization: This activity is part of the program of the Berkeley Thermodynamics Laboratory, Region II, U. S. Bureau of Mines. The Laboratory is situated on the University of California campus, Berkeley, Calif. Financial support is by annual appropriations from the Department of the Interior. The program has been directed since its start in

1931 by K. K. Kelley who, with the aid of a small staff, carries forward the compilation work. A valuable adjunct of the work is a related experimental program.

<u>Substances</u>: Inorganic compounds of interest in metallurgical and ceramic operations.

<u>Properties:</u> Those necessary for the computation of free energy values for metallurgical reactions. Free energies, entropies, heats of formation, high and low temperature heat capacities, and heats accompanying changes of state are the most important properties covered.

Sources of Data: Primarily the open literature; to a limited extent experimental studies on key substances.

Criticality: Available experimental and calculated values are evaluated and "best" values are presented. A critical discussion of the available data is frequently given. The demand for the publications of this project is a measure of the high regard in which it is held by workers in the field.

Use of Nomenclature, Symbols, Units, Physical Constants: Recommendations of authoritative national and international committees are followed.

<u>Currency</u>: Continuing coverage of the whole field of interest is not maintained. Selected topics are covered in individual bulletins which may be revised and extended from time to time.

Format: Earlier numbers of this paper-backed series were 5 3/4" x 9 1/8". A recent change has been made to 7 3/4" x 10 1/4". Data are presented both in text and in tables. The compounds are arranged alphabetically in each bulletin. Sources and other pertinent information are found in short textual passages. Useful empirical correlating equations, an author index, and bibliography are provided.

Publication and Distribution: CONTRIBUTIONS TO THE DATA ON THEORETICAL METALLURGY, I to XIII, have been published as Bureau of Mines Bulletins between 1932 and 1960. Some of the volumes are revisions of earlier ones. Those needed for a complete set of unrevised data are III, IV, V, VII, VIII, XI, XII, and XIII. The first six of these are out of print; Volumes XII and XIII may be obtained from the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C., for 45 cents and \$1.25, respectively. Revision of Volume XI is planned.

Contributions to the Data on Theoretical Metallurgy

- I. The Entropies of Inorganic Substances. K. K. Kelley, Bulletin 350, Bureau of Mines, 1932, 63 pp.
- II. High-Temperature Specific-Heat Equations for Inorganic Substances. K. K. Kelley, Bulletin 371, Bureau of Mines, 1934, 78 pp.
- III. The Free Energies of Vaporization and Vapor Pressures of Inorganic Substances. K. K. Kelley, Bulletin 383, Bureau of Mines, 1935, 132 pp.
- IV. Metal Carbonates, Correlation and Applications of Thermodynamic Data. K. K. Kelley and C. T. Anderson, Bulletin 384, Bureau of Mines, 1935, 73 pp.
- V. Heats of Fusion of Inorganic Substances. K. K. Kelley, Bulletin 393, 1936, 166 pp.
- VI. A Revision of the Entropies of Inorganic Substances -- 1935.
 K. K. Kelley, Bulletin 394, Bureau of Mines, 1936, 55 pp.
- VII. The Thermodynamic Properties of Sulphur and Its Inorganic Compounds. K. K. Kelley, Bulletin 406, Bureau of Mines, 1937, 154 pp.
- VIII. The Thermodynamic Properties of Metal Carbides and Nitrides. K. K. Kelley, Bulletin 407, Bureau of Mines, 1938, 66 pp.
 - IX. The Entropies of Inorganic Substances. Revision (1940) of Data and Methods of Calculation. K. K. Kelley, Bulletin 434, Bureau of Mines, 1948, 115 pp.
 - X. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for Inorganic Compounds. K. K. Kelley, Bulletin 476, Bureau of Mines, 1949, 241 pp.
 - XI. Entropies of Inorganic Substances. Revision (1948) of Data and Methods of Calculation. K. K. Kelley, Bulletin 477, Bureau of Mines, 1950, 147 pp.
- XII. Heats and Free Energies of Formation of Inorganic Oxides. James P. Coughlin, Bulletin 542, Bureau of Mines, 1954, 80 pp.

XIII. High-Temperature Heat-Content, Heat Capacity, and Entropy Data for the Elements and Inorganic Compounds. K. K. Kelley, Bulletin 584, 1960, 232 pp.

<u>Comment:</u> While most of the volumes of this project are out of print, they have received wide distribution and have served as a valuable source for other data compilations.

I-4. Manufacturing Chemists Association Research Project on Properties of Chemical Compounds

Organization: This project was established in 1955 at the Carnegie Institute of Technology in Pittsburgh, Pa. In early 1961 it was transferred to the Department of Chemistry, Agricultural and Mechanical College of Texas, College Station, Texas. It is sponsored and financed by the MCA. Until 1960 it was directed by Frederick D. Rossini who was succeeded by Bruno J. Zwolinski. The staff includes seven full- and part-time professional workers, plus supporting editorial and office help. A twelveman Advisory Committee provides guidance and liaison with industry. There has been continuous and steady effort from the project since its inception. Close contact is maintained with related experimental work.

<u>Substances</u>: All chemical compounds (except hydrocarbons) of interest to the chemical industry.

Properties: In time this project will cover the same properties as APIRP 44 (see I-1). At present, values are given for the following physical and thermodynamic properties—density; (dt/dp); refractive index; temperatures of boiling, melting, sublimation, and transition; vapor pressure; critical compressibility, density, pressure, temperature, and volume; heat and entropy of phase changes; change in heat capacity on phase changes. Property values are presented at standard reference points and selected intervals of the variables (temperature, pressure, etc.) over ranges dictated by probable use of the data and reliability of the extrapolation methods. (A spectroscopic program paralleling that of APIRP 44 began in 1959. See V-B-7, V-C-2, V-D-2, V-E-2, and V-F-2.)

Sources of Data: Original papers in the literature, available unpublished data, original calculations.

<u>Criticality</u>: The experienced staff carefully evaluates the available data. Where possible reliable correlation methods are used to create data for compounds not studied. Quasi-theoretical methods are used to extend the range of variables beyond the limits of convenient experimentation. After evaluation and correlation "best" values are selected. The methods of data treatment create internal consistency

within related bodies of information. The introduction to the publication includes a complete discussion of criteria used to evaluate, and methods used to create, data.

Use of Nomenclature, Symbols, Units, Physical Constants: New recommendations of authoritative national and international committees are adopted in ways and at times that will cause a minimum of change in the extensive tabulations.

<u>Currency</u>: Data for families of compounds are first brought up to date and then kept current. New groups of properties and series of compounds are added as needs arise and data become available. Revisions and additions are issued at regular intervals.

Format: All data are presented in tables on 8" x 10 1/2" loose-leaf sheets coded according to substance and property. No complete index is given but substances are logically arranged according to the Standard Order System which is based on the periodic table. Specific references (authors' surnames only) for each entry in the data tables are tabulated on separate sheets. Complete references are found in a general list of references.

Publication and Distribution: The covering title of the loose-leaf sheets is SELECTED VALUES OF PROPERTIES OF CHEMICAL COM-POUNDS. As of June 30, 1960 there were 577 valid sheets pertaining to physical and thermodynamic properties. New sheets are distributed semiannually by the Manufacturing Chemists Association, 1825 Connecticut Ave., N.W., Washington, D. C. Distribution of the sheets is made to three categories of recipients: (1) members of the Manufacturing Chemists Association - complimentary copies; (2) university departments, non-profit research institutions, government organizations, and independent free libraries - free copies, one set each; and (3) other interested persons - copies by sale. The sheets are sold, in complete sets only, at five cents per sheet.

I-5. Phase Diagrams for Ceramists

Organization: The American Ceramic Society and the National Bureau of Standards are the organizations most intimately connected with this compilation activity. Early compilers were F. P. Hall, Herbert Insley, and H. F. McMurdie, all of whom have been or are associated with NBS. Compilers of the most recent (1959) publication are E. M. Levin and H. F. McMurdie, both of NBS. Cooperation comes from other members of the NBS staff and from members of the American Ceramic Society who contribute diagrams, make suggestions, and note errors. In addition the Society provides editorial assistance. Recent compilations have been financed by a revolving fund created by the Board of Trustees of the Society from sales of previous issues.

<u>Substances:</u> Systems of interest to ceramists. Not included are some aqueous systems, some of those with volatile components, and systems covered elsewhere.

<u>Properties:</u> Phase diagrams for one-, two-, three-, and multi-component systems.

Sources of Data: World literature.

<u>Criticality</u>: Since, for each system, there are relatively few data from which to choose, the quality of the diagrams is variable. Outdated diagrams are replaced with later, more reliable ones, but there is no attempt to evaluate the accuracy of any diagrams. The diagrams, in general, are too small to permit values to be read off with any great accuracy. There has been no attempt to recalculate the drawings and make them uniform in statement.

Use of Nomenclature, Symbols, Units, Physical Constants: Units have not been conformed throughout, but this may be done in future publications.

<u>Currency:</u> Periodic supplements and revisions have been published. Another complete edition is in the planning stage; publication in about 1962 is expected.

Format: Two complete compilations with supplements were published in the "Journal of the American Ceramic Society" between 1933 and 1949. The latest compilation is in book form. Data are presented as phase diagrams which are sometimes accompanied by explanatory notes. The diagrams are grouped according to system composition and within each group are listed in order of increasing complexity. Author and system indexes are given. A complete reference is given below each diagram.

Publication and Distribution: Copies of the "Journal of the American Ceramic Society" containing the early compilations are no longer available. Over 8,000 copies of the 1949 edition were distributed. The latest compilation, PHASE DIAGRAMS FOR CERAMISTS, supersedes all previous ones. Part I (286 pp.) published in 1956 and Part II (153 pp.) published in 1959 are available from the American Ceramic Society, 4055 No. High Street, Columbus 14, Ohio, for \$10.00 and \$8.00, respectively.

I-6. Selected Values for the Thermodynamic Properties of Metals and Alloys

Organization: Organized in 1955, this project is situated in the Minerals Research Laboratory, Institute of Engineering Research, University of California, Berkeley, California. Ralph Hultgren supervises a staff of 3 to 7 professional workers. K. K. Kelley serves as a consultant. Sponsors in 1959 included 7 industrial firms, the American Iron and Steel Institute, and the U. S. Atomic Energy Commission.

Substances: All metallic elements and alloys.

Properties: Very complete thermodynamic data are given for both elements and compounds. Presented for the elements are heats, entropies, and free energy functions relative to standard states; heat capacity values for condensed and gas phases in tabular form at selected temperature intervals and as analytic functions; change of phase and vapor pressure data. For alloys the integral quantities given are the free energy, heat, excess free energy and excess entropy of formation. When possible, activities, activity coefficients, and relative partial molar quantities are given over a range of compositions. Presentation and discussion of all experimental data are very complete.

Sources of Data: Open literature; other compilations of critically evaluated data when available; to some extent, calculations by staff members of thermodynamic functions from spectral data.

<u>Criticality</u>: Numerous graphical and analytic methods are used to develop internally consistent and reliable values to meet the many situations found in alloy systems. Evaluation procedures are outlined in the introduction. In addition to presentation of "best" values, this project has the following secondary aims: (1) by estimates and extrapolations to provide useable data for partially studied systems; and (2) to reveal systems requiring further study because of insufficient or unreliable data.

Use of Nomenclature, Symbols, Units, Physical Constants:
These usages are clearly stated in the introduction and conform in most respects to those of long-established, related projects.

Format: The interim publication form is the $8 \ 1/2" \times 11"$ looseleaf sheet. For each system a discussion (Part I) is followed by tables of data and graphs (Part II). Table values are at intervals close enough for linear interpolation. The data sources are given in the discussion, and complete references are listed at the end (Part III). Each system is paginated by using the chemical symbols in alphabetical order followed by page numbers. Systems may be filed in alphabetical order.

Publication and Distribution: The covering title of the loose-leaf sheets is SELECTED VALUES FOR THE THERMODYNAMIC PROPERTIES OF METALS AND ALLOYS: Sheets for 126 metal or alloy systems have been distributed to date. Free distribution of sheets is made currently to laboratories needing them. Book publication is planned.

I-7. Selected Values of Chemical Thermodynamic Properties

Organization: This project is in the Chemistry Division of the National Bureau of Standards. It has functioned since 1940 although the intensity of effort varies from year to year. The director since 1950 has been Donald D. Wagman who succeeded Frederick D. Rossini on the latter's resignation from NBS. This NBS activity has been supported in part by the Office of Naval Research and the U. S. Atomic Energy Commission.

<u>Substances</u>: The program includes all elements, inorganic compounds, and C_1 and C_2 organic compounds. Data for a few ionic species are given. Coverage in recent years has narrowed to selected subject areas. There are plans to revive the original broad coverage and possibly to extend it to cover selected groups of organic compounds with more than two carbon atoms.

<u>Properties:</u> The following three categories of properties are presented -- (1) basic thermodynamic properties at 25° C (heat, free energy, equilibrium constant, and entropy of formation; heat capacity); (2) temperature, heat and entropy of phase changes; (3) thermodynamic properties to 5000° K (heat, free energy, and equilibrium constant of formation; free energy function; heat content function; entropy; heat content; and heat capacity). For solutions of important soluble salts, thermodynamic properties are given at concentrations from near saturation to infinite dilution.

Sources of Data: The main source of information is published literature. Unpublished research reports are used to a limited extent.

<u>Criticality</u>: The experienced staff evaluates all literature data and uses standard procedures to yield a body of internally consistent data. "Selected" values are given. The 25° values presented by this project constitute a base on which all thermodynamicists depend.

Use of Nomenclature, Symbols, Units, Physical Constants: In general, usages prescribed by NRC, IUPAC, and other authoritative committees are followed.

<u>Currency</u>: Coverage of the literature to 1950 is good but recently wide areas have been neglected in favor of selected special topics. Reestablishment of currency is planned. (See Publication and Distribution.)

Format: Tabular arrangement of data on an 8" x 10 1/2" page is the form of presentation. The tables are grouped into Series I (25° properties), Series II (change of state properties), and Series III (thermodynamic properties at even temperatures up to 5000° K). No complete index is given but substances are logically arranged according to the Standard Order System which is based on the periodic table. Specific references (authors' surnames only) for each entry in the data tables are tabulated on separate sheets. Complete references are found in a general list of references.

Publication and Distribution: Series I, II, and III data were originally disseminated on loose-leaf sheets. Series I and II sheets valid as of February 1, 1952, and complete references were consolidated and published as NBS Circular 500, SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES (iv + 1268 pp.). Circular 500 is out of print; publication of a revision in about 1962 is expected. Many of the Series III sheets are out of print; separate publication of this series is planned.

I-8. Thermodynamic Properties of Selected Minerals at High Temperatures

Organization: This new project is a part-time activity of several staff members of the Geophysics Branch of the Geological Survey, Silver Spring, Md. Information about the project may be obtained from Richard A. Robie.

<u>Substances:</u> Minerals commonly found in natural rocks and related inorganic substances.

<u>Properties:</u> Heat content, entropy, and free energy function are presented at intervals of 100° up to 1000-2000°K. Also given are heats and free energies of formation of each compound from the elements and the corresponding oxides.

<u>Criticality:</u> The project is still developing its methods and is adopting desirable features from other similar, established projects. Care is being taken to insure internal consistency.

Sources of Data: Data from the literature and other compilations. Standard states and thermodynamic properties of the elements are taken from THERMODYNAMIC PROPERTIES OF THE ELEMENTS by D. R. Stull and G. C. Sinke (No. 18 of Advances in Chemistry Series of the American Chemical Society).

Use of Nomenclature, Symbols, Units, Physical Constants: Usage is expected to conform to that of other established projects.

<u>Currency</u>: The beginning effort is not comprehensive and complete. One publication a year for the next five years is expected.

Format: Data are presented in tables. Pertinent references are given as footnotes to each table.

<u>Publication and Distribution:</u> Data for the first group of compounds are in process of publication in a Geological Survey Bulletin. The Bulletin will bear the number 1083-E.

II. CRYSTALLOGRAPHIC AND MINERALOGICAL PROJECTS

II-1. The Barker Index of Crystals

Organization: In this publication measurements of interfacial angles of crystals are used to classify and identify chemical substances. T. V. Barker, who developed the classification-angle system, was about to begin the systematic compilation of the index when he died in 1931. The compilation work was undertaken by a number of interested crystall-ographers in the Department of Mineralogy of the University Museum at Oxford. Since 1948 the working headquarters has been the Department of Geology and Mineralogy. Numerous cooperating individuals in Great Britain, Holland, the United States, and Belgium have contributed editorially or by making calculations. Great interest and practical help have been given by the Barker Index Committee. Financial and material help have come from academic, governmental, and industrial organizations in England and Holland. Editors for Volumes I and II were M. W. Porter and the late R. C. Spiller, both of Oxford University. A third volume remains to be published.

<u>Substances</u>: Volume I deals with 2991 compounds belonging to the tetragonal, hexagonal and trigonal, and orthorhombic systems; and Volume II, with about 3500 monoclinic substances. Volume III, in preparation, will treat the anorthic compounds described in Groth's CHEMISCHE KRYSTALLOGRAPHIE.

<u>Properties:</u> The Barker system is based on the use of the smallest number of interfacial angles necessary for indexing purposes. Other morphological, physical, and optical property values are also given.

Sources of Data: The index is essentially a new treatment of previously compiled morphological data. Most of the data used are from Groth's CHEMISCHE KRYSTALLOGRAPHIE.

<u>Criticality</u>: Every calculation has been made independently by two workers and checked by one of the editors.

Use of Nomenclature, Symbols, Units, Physical Constants: Accepted crystallographic symbolism has been used; other symbols related to the index necessarily have been introduced.

<u>Currency</u>: This publication covers the old literature (Groth); there is no mechanism for keeping the volumes up to date.

Format: The publication form is that of clothbound books. The data are presented in lists and tables. Part 1 in both volumes is labeled "Introduction and Tables." The tables include those for the classification angles, refractive indices, and melting points of the various types of crystals. Part 2 of Volume I and Parts 2 and 3 of Volume II contain the crystal descriptions. These are grouped into sections according to the crystal system, and within each section compounds are arranged in the same order as in Groth's CHEMISCHE KRYSTALLOGRAPHIE. An alphabetical list of chemical and mineralogical names with reference numbers enables one to find a particular crystal description. References to the data sources are given in the crystal descriptions.

Publication and Distribution: The BARKER INDEX is published for the Barker Index Committee by W. Heffer & Sons, Ltd., 3-4 Petty Cury, Cambridge, England. Volume I containing Parts 1 and 2 was published in 1951; Volume II, in three parts, in 1956. The two volumes are available from the publisher for \$16.80 and \$28.00, respectively.

II-2. Crystal Data

Organization: The present edition of CRYSTAL DATA was written by J. D. H. Donnay, the Johns Hopkins University, Baltimore, Md. (Part II) and Werner Nowacki, University of Berne, Switzerland (Part I) with the collaboration of Gabrielle Donnay, U. S. Geological Survey, Washington, D. C. Many collaborators in the United States and Switzerland helped in collecting and assembling data, in making calculations, and in editing. Support came from academic and industrial groups in these two countries. The Geological Society of America gave a grantin-aid to complete the work and bore the expenses of publication. Preparation of a second edition is in progress under the sponsorship of the Crystal Data Committee of the American Crystallographic Association. Coeditors are J. D. H. Donnay, G. E. Cox of Leeds University, and Olga Kennard of the National Council for Medical Research, London. Financial grants have been received from the National Science Foundation and the (British) Institute of Physics for the compilation work and the publication costs. The continuity of the project is suggested by plans for an eventual third edition.

<u>Substances</u>: Elements, alloys, inorganic and organic compounds. (Metal data will not be included in the second edition, since these have been collected independently by W. B. Pearson, National Research Council, Ottawa, and published as A HANDBOOK OF LATTICE SPACINGS AND STRUCTURES OF METALS AND ALLOYS by Pergamon Press.)

<u>Properties:</u> Crystallographic data resulting mainly from X-ray and electron diffraction measurements are presented. Cell dimensions, number of formula units per cell, space group, and specific gravity are given for all substances. For some substances, auxiliary properties such as the melting point are given.

Sources of Data: Part I of the present edition covers the literature to mid-1948; Part II, up to the end of 1951. Much of the material comes directly from secondary sources such as STRUKTURBERICHT.

<u>Criticality:</u> The vast number of compounds to be covered, the limited resources to do the job, and the immediate need for this type of compilation precluded a thorough evaluation of all available data in the present edition. Future editions may be more critical.

Use of Nomenclature, Symbols, Units, Physical Constants: Since Parts I and II were prepared independently, the abbreviation schemes and the chemical symbols used differ in the two parts. The second edition should have greater uniformity.

<u>Currency</u>: A second edition is in preparation, and there are long range plans for a third.

Format: Data in the present edition are presented in tables and lists. Part I deals with the classification of crystalline substances by space groups and is not a numerical data compilation. The compounds are divided according to composition into seven categories. Part II contains determinative tables for the identification of crystalline substances. These are arranged according to crystal system. There are formula and name indexes covering both parts. References for Part I are given at the end and for Part II in the tables.

Publication and Distribution: The present edition of CRYSTAL DATA (ix + 719 pp.), published in 1954 as Memoir 60 of the Geological Society of America, is now out of print. The manuscript of the second edition will probably be ready by the end of 1960.

II-3. Crystal Structures

Organization: The author of CRYSTAL STRUCTURES is Ralph W. G. Wyckoff, University of Arizona, Tucson, Arizona. The first section of this publication appeared in 1948 and the last supplement in 1960. Though now complete, the publication is included in this directory because of its importance and because of the long-term nature of its preparation.

<u>Substances:</u> Elements, inorganic and organic compounds (no alloys).

<u>Properties:</u> The data presented are derived almost entirely from X-ray diffraction measurements and include atomic coordinates, cell dimensions, and atomic and ionic radii.

Sources of Data: Published literature.

<u>Criticality</u>: The aim was to state the results of <u>all</u> available determinations of atomic positions in crystals. Presumably the tabulated data are best available values. The critical comments in the textual sections of this publication are invaluable.

Use of Nomenclature, Symbols, Units, Physical Constants: The terminology used conforms to that of INTERNATIONALE TABELLEN ZUR BESTIMMUNG VON KRISTALLSTRUKTUREN.

<u>Currency</u>: During the years of publication, supplement and replacement sheets were issued periodically. Coverage of the literature extends through 1954 and includes some 1955 references. It is to be hoped that some way will be found to keep this important work current.

Format: The publication form is that of loose-leaf sheets (7 3/4" x 9 3/4") contained in binders. The book is divided into chapters and in each chapter the material is grouped into Text, Tables, Illustrations, and Bibliography. Each group is paginated separately; numbers sometimes followed by letters are used so that insertions can be made. Inorganic structures are found in Chapters II-XII, organic structures in Chapters XIII-XV. Within each chapter an effort has been made to group together those crystals with similar structures. There are three indexes, i.e., an inorganic formula index, a mineralogical name index, and a name index to organic compounds.

Publication and Distribution: Publisher of CRYSTAL STRUCTURES is Interscience Publishers, 250 Fifth Avenue, New York 1, N. Y. The work consists of four sections and 5 supplements. Price of the complete work including all necessary binders is \$148.50.

II-4. Dana's System of Mineralogy

Organization: Six editions of James Dwight Dana's SYSTEM appeared between 1837 and 1892. In 1915 Edward S. Dana, editor of the sixth edition, asked W. E. Ford of Yale University to prepare a seventh edition of his father's work. A number of people became involved in the preparation but work was slow until 1937. In that year a grant was obtained from the Penrose Fund of the Geological Society

of America to finance additional full-time workers. Money was also advanced by the publishers, John Wiley & Sons, Inc. Volume I was completed in 1941 and published in 1944. The editors of this volume and Volume II were the late Charles Palache, Clifford Frondel, and the late Harry Berman, all of Harvard University. Work on Volume II was begun in 1941, interrupted by the war in 1942, and resumed in 1945. The volume was completed in 1950 and published in 1951. A supplementary grant from the Geological Society of America helped finance its publication. Besides the editors there were many contributors in the United States and Great Britain to Volumes I and II. W. E. Ford, for example, continued to supply data on the occurrence of minerals until his death in 1939. Volume III is nearing completion and there are plans to revise Volume I. The project is currently supported by Harvard University.

Substances: Minerals.

<u>Properties:</u> Crystallographic, physical, optical, and chemical properties. The crystallographic data given include interaxial angles and unit cell dimensions; the physical property values include hardness, melting point, and specific gravity.

Sources of Data: Almost entirely original articles in journals; abstracts and other compilations on rare occasions when original papers are not available.

<u>Criticality</u>: All information is carefully appraised and uncertain facts are designated by (?). An authentic diffraction pattern is always obtained and optical properties are frequently checked.

Use of Nomenclature, Symbols, Units, Physical Constants: Recommendations of international authorities, such as the International Union of Crystallography, are followed. There is a complete synonymy at the beginning of each species description.

<u>Currency</u>: Currency in the usual sense cannot be maintained in an undertaking of this sort.

Format: The data are presented in text and tables in bound volumes. Volume I of the seventh edition contains an introduction and data for eight classes of minerals; Volume II contains data for forty-two classes. References are given at the end of each mineral description and a general index is given at the end of each volume. There will be a comprehensive index in Volume III covering all three volumes.

Publication and Distribution: Volume I (xiii + 834 pp.) of the seventh edition of DANA'S SYSTEM OF MINERALOGY was published in 1944 and Volume II (xi + 1124 pp.) in 1951 by John Wiley & Sons, Inc., New York, N. Y. (The association of Wiley & Sons with the Dana Mineralogies dates back to 1844 when they published the second edition of the SYSTEM.) The two volumes are available from the publisher for \$14.00 and \$16.00, respectively.

II-5. The Groth Institute

Organization: "The Groth Institute," which was established in 1958, is a group activity affiliated with the Physics Department of The Pennsylvania State University, University Park, Pa. Ray Pepinsky is the Director. The Institute derives its name from Paul von Groth's CHEMISCHE KRYSTALLOGRAPHIE, a five-volume work which appeared between 1906 and 1919. The resident staff is large and consists of professional assistants, graduate students, abstractors, librarian, technical editor, machine operators, secretarial help, and others. There are also corresponding members and outside advisory groups. The Air Force Office of Scientific Research has provided financial assistance in the early stages of the Institute's program.

<u>Substances:</u> All crystalline substances and other solid-state materials.

<u>Properties:</u> The aim is to collect a very broad range of physical, chemical, morphological, and structural data for crystals on an encyclopedic scale and to seek all possible useful and revealing correlations of properties with internal structure.

Sources of Data: The first stage of operation has centered on the literature imaging of critical or summarizing tabulations such as the Barker Index. Coverage of primary literature will follow. Unpublished data will be available to the Groth institute from cooperating groups and individuals.

<u>Criticality</u>: Critical evaluation of all data compiled is not a primary aim of this project. However, the proposed correlation of the many interrelated properties of crystals will reveal discrepancies in the recorded data and suggest areas for reinvestigation. In addition, the availability of computers will permit recalculation and refinement of much structural information.

Use of Nomenclature, Symbols, Units, Physical Constants: For punched-card or tape storage of information all literature values must be conformed to a common language. In this way a degree of unification of nomenclature, symbols, and units will be realized.

<u>Format:</u> All data will be recorded on punched cards and tape for high speed correlation and retrieval. Information will also be available in tabular form on automatic print-out sheets from machines.

Publication and Distribution: No attempt will be made to publish the mass of experimentally determined property values or the data that may be derived by calculation. Instead, monographs and summaries will be produced by automatic print-out to satisfy special needs. In about 1964 work will begin on a new edition of Groth's encyclopedia. This revision will bear the title GROTH'S ENCYCLOPEDIA OF CHEMICAL AND PHYSICAL CRYSTALLOGRAPHY, REVISED EDITION. The store of information in the Institute repository, which is available to other scientists, will serve as valuable source material to others engaged in more conventional compilation activities.

II-6. Joint Committee on Chemical Analysis By X-ray Diffraction Methods

Organization: This committee is made up of representatives from the following organizations: American Society for Testing Materials, American Crystallographic Association, (British) Institute of Physics, and the National Association of Corrosion Engineers. The aims of the committee are to collect, edit, publish, and distribute powder diffraction data in suitable form to serve as references for the identification of crystalline substances from their diffraction patterns, and to sponsor suitable projects for the improvement and development of data for such purposes. Chairman of the Committee is H. W. Rinn, the Dow Chemical Co., Midland, Mich. J. V. Smith, Department of Geology, University of Chicago, is the current editor-in-chief of the X-RAY POWDER DATA FILE. L. G. Berry, Queen's University, Canada (minerals); Benjamin Post, Polytechnic Institute of Brooklyn (organic and inorganic substances); and Sigmund Weissmann, Rutgers University (metals and alloys) became associate editors in 1953. The committee finances research associateships at the National Bureau of Standards as part of an NBS-supported program for the improvement of the powder data file. In the Constitution and Microstructure Section of NBS, which is headed by H. F. McMurdie, conflicting data in the card file are reviewed, correct patterns are selected, and new patterns are measured. The great value of the data file as an analytical tool insures the continuity of this project. The file has been in existence since about 1941.

Substances: Solid materials of interest to science and industry.

Properties: Powder patterns (by more than one technique).

Sources of Data: NBS measurements; measurements made under the direction of editors Smith, Berry, Post, and Weissmann; measurements made under the direction of A. J. C. Wilson, University College, Cardiff, Wales, and P. M. de Wolff in Delft; data from the literature and from individual investigators.

<u>Criticality</u>: The editors decide on the suitability of new data for inclusion in the file. A system of editing, recently introduced, results in a double and triple check on the data. Under the NBS program, most of the multiple entries for particular substances have been supplanted by single standard patterns measured on very pure samples. Professor Wilson's group also checks existing data.

<u>Currency</u>: Efforts are made by the group to generate new data. Old data, when of inferior quality, are replaced as quickly as possible.

Format: The X-ray diffraction powder patterns are presented on (3" x 5") plain cards suitable for manual operation, (4" x 6") Keysort cards, and standard IBM cards. The cards are arranged according to the d-values of the strongest three lines. Line intensities are given, and lattice constants, space group, etc. are presented if available. A cumulative index in book form is periodically revised to include each new section as it is added. Data obtained from patterns measured at NBS are published separately in paper-covered booklets. In these booklets ASTM card data for a given substance are tabulated for comparison with other values from the literature and with the values obtained at NBS for the same substance.

Publication and Distribution: Ten sections (nearly 10,000 cards) of the X-RAY POWDER DATA FILE have been published by ASTM. These sections may be purchased, separately if desired and in any of the available card forms, from the American Society for Testing Materials, X-Ray Dept., 1916 Race St., Philadelphia 3, Pa. The total price of the 10 sections is \$1,110.00 for the plain cards, \$1,730.00 for the keysort cards, and \$405.00 for the IBM cards. Additional decks are available at reduced prices. The cumulative index is available gratis with orders for any portion of the Plain or Keysort Decks. The first five sections of data have been reissued in 1960, both in book and card forms. The new material contains numerous additions and corrections resulting from a comprehensive review by the editors. The publication STANDARD X-RAY DIFFRACTION POWDER PATTERNS has been published by NBS as Circular 539. Volumes 1 through 10 (716 pp.) have appeared between 1953 and 1960. These may be purchased from the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C. for a total of \$4.30.

II-7. Structure Reports

Organization: STRUCTURE REPORTS is an annual collection of abstracts of a special type. Structural information only is extracted from articles on crystallography which may or may not contain other material. Frequently the reports are amplified by the addition of values derived from the data originally reported. This publication takes the place of STRUK-TURBERICHT, which was published in seven volumes from 1913 through 1939. Work on STRUCTURE REPORTS began in 1949. It is edited by A. J. C. Wilson, University College, Cardiff, Great Britain, and prepared under the guidance of The Commission on Structure Reports of the International Union of Crystallography. There are section editors for metals, inorganic compounds, and organic compounds. Until about 1954 financial support was received from UNESCO, the national committees for crystallography in Great Britain and the United States, de Nederlandse Organisatie voor Zuiver Wetenschappelijk Onderzoek, and other organizations in these three countries. The volumes, from the fifteenth on, are to be sold at prices designed to recover the cost of production.

Substances: Metals, inorganic and organic compounds.

<u>Properties:</u> The data presented are derived primarily from X-ray diffraction measurements. Investigations of texture, papers containing powder data, and electron-diffraction studies are reported when of structural interest. Unit cell dimensions, space groups, atomic positions and parameters, interatomic and intermolecular distances are given.

Sources of Data: Published papers.

<u>Criticality</u>: This publication is intended as a source of precise information on <u>all</u> determinations of crystal structures. It aims at giving a complete account of the papers reported. However, detailed assessments of each structure are made and critical comments are inserted by the abstractors and editors when necessary.

<u>Currency</u>: In order to give priority to newer work, volume 11, published in 1951 and covering the years 1947-48, was the first to appear. Since then the publication order has been volumes 12, 10, 13, 9, 8, 15, 14, and 16. Volume 8 bridged the gap of the war years and thus follows volume 7 of STRUKTURBERICHT. Volume 15, published in 1957 and covering the literature for 1951, represents the start of an effort to establish currency.

Format: STRUCTURE REPORTS is published in book form. Data are presented in tables and text. The volumes are divided into three main sections: Metals, Inorganic Compounds, Organic Compounds. In

the Metals section the arrangement is alphabetical. Reports in the other sections are roughly in the order of increasing complexity of composition. Within each volume there are subject, formula, and author indexes and an index of carbon compounds. Volume 14, which contains a few supplementary reports for the period 1940-50, is a cumulative index for volumes 8 through 13.

Publication and Distribution: Volumes 8 through 16 of STRUCTURE REPORTS (about 4500 pp.) have been published for the International Union of Crystallography by N. V. A. Oosthoek's Uitgevers Mij in Utrecht. Prices range from \$11.25 for the small index volume to \$38.00 for Volume 16.

III. NUCLEAR PHYSICS PROJECTS

III-1. Neutron Cross Sections (Brookhaven)

Organization: Brookhaven National Laboratory, Upton, New York, is the site of this program. Sponsored and financed by the Atomic Energy Commission, the work has been carried on as a part-time activity of two or three professional physicists with editorial and secretarial help furnished by AEC. The program was coordinated by Donald J. Hughes until his death in April 1960.

Substances: All nuclides.

<u>Properties:</u> Thermal cross sections, resonance parameters, cross section curves, angular distributions.

Sources of Data: Literature values and unpublished ones available to the authors.

<u>Criticality</u>: The publications of this project are intended to serve primarily the needs of reactor physicists and engineers. Where possible "best values," based on an evaluation of all available data by the compilers, are given with estimated errors. No description of the evaluation methods is given.

Use of Nomenclature, Symbols, Units, Physical Constants: An attempt is made to put quantities in consistent units.

<u>Currency</u>: Supplements are issued and revisions made. Unpublished contributions from individuals result in the presentation of many very recent values.

Format: The publication form is that of paper-covered books. Two page sizes have been used, $10 \ 1/4$ " x $14 \ 1/2$ " and $8 \ 3/8$ " x $10 \ 3/4$ ". Data are presented in tables and graphs. The over-all arrangement of data is by property and, under each property, data are given in the order of increasing atomic numbers and masses. Sources of data are identified in the tables and curves by an abbreviation of the laboratory and a number referring to a general list of references following the data presentation.

<u>Publication and Distribution:</u> The publications of this project have appeared in the following chronological order:

AECU 2040, May 1952.

BNL 325, NEUTRON CROSS SECTIONS, July 1955, v + 328 pp. BNL 400, NEUTRON CROSS SECTIONS - ANGULAR DISTRIBUTIONS, June 1956, 102 pp.

Supplement No. 1 to BNL 325, January 1957, xxvii + 129 pp. BNL 325, 2nd edition, NEUTRON CROSS SECTIONS; July 1958, v + 373 pp.

Supplement No. 1 to the 2nd edition of BNL 325, January 1960, iv + 129 pp.

BNL 325 and its supplement may be purchased from the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C. for \$4.50 and \$2.00, respectively, and BNL 400 from the Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C., for 50 cents.

III-2. Neutron Cross Sections (UCRL)

Organization: This program is carried out at the University of California Lawrence Radiation Laboratory, Livermore, Calif., under the direction of Robert J. Howerton of the Theoretical Physics Division. The Atomic Energy Commission provides financial support.

Substances: All nuclides.

<u>Properties:</u> Data for total and reaction neutron cross sections in the energy range from 0.001 through 14.5 Mev have been presented. Subsequent volumes are planned that will extend the energy range. A tabulation of differential neutron cross sections is in press.

Sources of Data: Journals, AEC report literature, and private communications.

<u>Criticality</u>: In the first three volumes of tables published, no selection of best values was made; essentially all available experimental data were presented. In a complete revision of these volumes an effort was made to eliminate clearly superseded data. A brief discussion of the methods used to select data is given in the introduction.

Use of Nomenclature, Symbols, Units, Physical Constants: Symbolism in this field is not well established. A notation system has been used that, it is hoped, is the least ambiguous possible.

<u>Currency:</u> Replacement sheets, published annually as addenda, are planned.

Format: Loose-leaf sheets are contained in plastic-covered binders. Part I, entitled TABULATED NEUTRON CROSS SECTIONS, contains three volumes and is completely tabular. Volume I of Part I contains the data for $_1\text{H-}_{22}\text{Ti}$; Volume II, data for $_{23}\text{V-}_{50}\text{Sn}$; and Volume III, data for $_{51}\text{Sb-}_{95}\text{Am}$. No index is provided since the material is arranged in the order of increasing atomic number. Sources of data are identified in the tables by numbers referring to complete reference lists at the back of each volume. Part II, Volume I has the title SEMI-EMPIRICAL NEUTRON CROSS SECTIONS, 0.5-15 MEV. In this publication a discussion section is followed by cross-section energy curves for $_1\text{H}^1$ - $_{94}\text{Pu}^{239}$. Since the data plotted are taken from the Part I tables, no references to original sources are given.

Publication and Distribution: TABULATED NEUTRON CROSS SECTIONS, and SEMI-EMPIRICAL NEUTRON CROSS SECTIONS, were published by the U. S. Atomic Energy Commission. The former bears the designation UCRL-5226 and the latter, UCRL-5351. The first edition of UCRL-5226 was published May 1958 and a revision in October 1959; UCRL-5351 (274 pp.) was published November 1958. These may be purchased (the volumes of Part I separately, if desired) from the Office of Technical Services, U. S. Department of Commerce, Washington, D.C. Prices are as follows: UCRL-5226, Vol. I, \$6.00, Vol. II, \$6.00, Vol. III, \$4.00; UCRL-5351, \$4.00. TABULATED DIFFERENTIAL NEUTRON CROSS SECTIONS will be designated as UCRL-5573.

III-3. Nuclear Data Project

Organization: This project was established in 1948 at the National Bureau of Standards in Washington, D. C. In 1953 the group was transferred to the National Academy of Sciences—National Research Council, Washington 25, D. C. Administratively it is under the Division of Physical Sciences of NAS—NRC and is financed by the Atomic Energy Commission. A full-time professional staff of five or six is under the direction of Katharine Way.

Substances: All nuclides.

Properties: The number of properties covered has increased over the years. The data currently presented in the NUCLEAR DATA SHEETS are of the following types: ground state (covering data on nuclear angular momentum, nuclear magnetic dipole moment, nuclear electric quadropole moment, abundances, and thermal neutron absorption cross sections), ground-state decay, metastable-state decay, reaction data, mass-spectrometer data, and mass links.

Sources of Data: Pertinent journals and abstracts.

<u>Criticality:</u> All experimental results are reported but critical comments are given. When decay schemes are drawn one value is usually selected, although sometimes alternative schemes are presented. Discrepancies are emphasized in order to stimulate research. "Adopted" values are given when this is justified by the available scientific evidence.

Use of Nomenclature, Symbols, Units, Physical Constants: In general the group follows the recommendations of international committees.

Currency: Additions and revisions are issued at regular intervals.

Format: Many of the numerical data are presented in tabular form. Wherever possible, decay schemes or level diagrams have been drawn that give graphical representation to a number of results. The two current continuing publications of the group, the NUCLEAR DATA SHEETS and the annual cumulations, are complementary to each other. In the former the arrangement of material is by nucleus and in the latter it is by property. Each loose-leaf sheet (8 1/2" x 11") of the first named publication contains the cumulated data, with references, for a particular nucleus. When new information becomes available on a nucleus for which a sheet has already been prepared, a "replacement" sheet is issued. The most recent version of the annual cumulations, the 1959 NUCLEAR DATA TABLES, is a paperbacked book, 7.7/8" x 10.1/4". It contains cumulated lists on properties such as spins, moments, abundances, and reaction energies.

<u>Publication and Distribution:</u> The numerical data publications of this project have appeared in the following chronological order:

- (1) NBS Circular 499, NUCLEAR DATA. A COLLECTION OF EXPERIMENTAL VALUES OF HALF-LIVES, RADIATION ENERGIES, RELATIVE ISOTOPIC ABUNDANCES, NU-CLEAR MOMENTS AND CROSS SECTIONS, September 1950, iv + 309 pp.
- (2) Supplement 1 to Circular 499, April 1951, iv + 56 pp.
- (3) Supplement 2 to Circular 499, November 1951, ii + 63 pp.
- (4) Supplement 3 to Circular 499, June 1952, ii + 66 pp.
- (5) NEW NUCLEAR DATA, ANNUAL CUMULATIONS, issues 24B of Volumes 6 through 10 of "Nuclear Science Abstracts," December 1952, 1953, 1954, 1955, and 1956.

- (6) NUCLEAR DATA CARDS, 1954-1957.
- (7) TID-5300, NUCLEAR LEVEL SCHEMES -- A=40 TO A=92, September 1955, xx + 221 pp.
- (8) 1957 CUMULATION, NEW NUCLEAR DATA, 167 pp.
- (9) NUCLEAR DATA SHEETS, January 1958--
- (10) 1959 NUCLEAR DATA TABLES, April 1959, viii + 151 pp.
- (11) 1960 NUCLEAR DATA TABLES, Parts 1-4, 1960

The data contained in publications (1) through (4) and (6) have been superseded by later publications. The copies of "Nuclear Science Abstracts" containing the ANNUAL CUMULATIONS for 1952 through 1956 are now out of print. The NUCLEAR DATA SHEETS are available by subscription from the Publications Office, National Academy of Sciences-National Research Council, Washington 25, D. C. The annual subscription price is \$17.00 for paper stock and \$20.00 for card stock. Publications (8), (10) and (11) may be purchased from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. Prices are \$1.25 for (8), \$1.00 for (10) and \$1.25 for Part 3 of (11); prices for parts 1, 2, and 4 of (11) were not available at the time of writing. Two other publications of the Nuclear Data Project, which are not numerical data compilations, are:

- (12) NUCLEAR THEORY INDEX CARDS, January 1958--
- (13) A DIRECTORY TO NUCLEAR DATA TABULATIONS, January 1958, xiii + 185 pp.
- K. Way is coauthor of another short numerical data compilation:
 - (14) RADIATIONS FROM RADIOACTIVE ATOMS IN FREQUENT USE, February 1959, xii + 75 pp.

Publication (12) may be purchased on a subscription basis from the NAS-NRC Publications Office. The 1958 and 1959 back issues are \$5.00 each and the 1960 subscription price is \$6.00. Publications (13) and (14) are available from the Superintendent of Documents for 70 cents and 55 cents, respectively.

IV. THERMOPHYSICAL PROJECTS

IV-1. Thermophysical Properties of Cryogenic Materials

Organization: This new activity is part of a broad data collection program of the Materials Central, Wright Air Development Division, Air Research and Development Command, United States Air Force. WADD, which conducts and sponsors numerous activities in cryogenic engineering, contracted with the National Bureau of Standards to collect and compile data on the thermophysical properties of materials used in low temperature applications. Work began early in 1958 at the Cryogenic Engineering Laboratory of NBS in Boulder, Colorado. Victor J. Johnson, Chief of the Cryogenic Data Center, serves as general editor. In the initial stages of this program qualified senior staff members of the Laboratory made literature searches and evaluated the data as a part-time activity. Student aids helped to prepare detailed data sheets and to identify references in the literature. Future phases of the work will be carried on by at least one full-time experienced person with the aid of other staff members for review and criticism of the data.

<u>Substances:</u> Initially, ten of the most common cryogenic fluids and a number of solids used at low temperatures.

Properties: Thermophysical properties in the temperature range from near absolute zero up to 110°K, or occasionally up to 300°K. In Phase I of the program the following properties are given for fluids: density, expansivity, thermal conductivity, specific heat and enthalpy, transition heat, phase equilibria, dielectric constant, adsorption, surface tension, and viscosity. For solids the properties given are: thermal expansion, thermal conductivity, and specific heat and enthalpy. Phase II of the program will cover eight additional properties.

Sources of Data: Published literature.

<u>Criticality</u>: Summarizing graphs of most probable values are given for use of the design engineer. Experimental or smoothed values from the primary source(s) are tabulated. Also given are other references of merit and brief comments concerning the data. Occasionally, alternate values from other references are tabulated for comparison.

Use of Nomenclature, Symbols, Units, Physical Constants: Both metric and engineering units are used.

Currency: There are plans to issue revision and addition sheets.

Format: Loose-leaf sheets (8 1/4" x 10 3/4") are assembled in book form under paper covers. Phase I data are contained in three parts: Part I-Properties of Fluids, Part II-Properties of Solids, Part III-Bibliography of References. The primary arrangement is by property rather than material. Each data sheet is complete and has a code number corresponding to the property and material classification. Sheets are placed in the compendium in ascending order of code number.

Publication and Distribution: Phase I data were issued in late 1960 as WADD Technical Report 60-56. The covering title is COMPENDIUM OF THE PROPERTIES OF MATERIALS AT LOW TEMPERATURES; PHASE I. The report is available by purchase from the Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C.

IV-2. Thermophysical Properties of Solid Materials

Organization: This compilation activity is another part of the program of the Materials Central, Wright Air Development Division, Air Research and Development Command. It is carried out under contract with the United States Air Force in the Heat and Mass Transfer Section of the Fluid Dynamics and Systems Research Division of the Armour Research Foundation, Chicago, Ill. The study, compilation and evaluation phases are performed by a staff of about eight. Literature searching was done by members of the Technical Information Research Section. Members of other departments of ARF act as advisors.

<u>Substances</u>: Elements, alloys, ceramics, cermets, and intermetallics melting above 1000° F; polymeric and composite materials of any melting temperature.

<u>Properties:</u> Density; melting point; latent heat of fusion, vaporization, and sublimation; crystal habit and transformation temperature; specific heat; thermal conductivity; thermal diffusivity; emissivity, reflectivity; linear thermal expansion; vapor pressure; electric resistivity.

Sources of Data: Original data published during the period 1940-1957, inclusive, on the thermophysical properties of solid materials. In some instances, where data are not available from the current survey, density and melting point information is taken from secondary (non-original) sources.

<u>Criticality</u>: For density and heats and temperatures of phase changes "best values" are selected from available data. For the other properties, tables of values are compiled at selected temperature intervals from smooth curves fitted to available data.

Use of Nomenclature, Symbols, Units, Physical Constants: Data are given in both metric and engineering units.

<u>Currency</u>: A mechanism is planned for the inclusion of new data and the substitution or deletion of old data.

Format: In a preliminary report, data are presented on 8 1/2" x 11" sheets in graphical and tabular form with all entries annotated. Materials are arranged in accordance with a Materials Index based on the chemical composition of materials. (The Materials Index also serves as a code for a punched card system.) For a given material, data for the several properties are arranged according to a definite plan. Each sheet is identified by a number, the first two digits of which give the year the sheet was prepared. Data sources are identified by hyphenated numbers which indicate the year of publication and refer to a List of References at the back of the volume. An alphabetical Author Index is cross-referred to the List of References and the body of data.

Publication and Distribution: WADC Technical Report 58-476, THERMOPHYSICAL PROPERTIES OF SOLID MATERIALS, by Alexander Goldsmith and Thomas E. Waterman was issued in October 1958 (about 400 pp.) This report covers the work carried out from June 1, 1957, to July 31, 1958, and is preliminary in nature. It is available for \$6.00 from the Office of Technical Services, U. S. Department of Commerce, Washington, D. C. Pergamon Press will publish the final compilation in early 1961. The complete work will consist of four volumes containing 3750 pages of data and a fifth appendix volume containing the List of References and indexes.

IV-3. Thermophysical Properties Research Center (TPRC)

Organization: This center was established in 1957 and operates within the administrative framework of the School of Mechanical Engineering, Purdue University. The organization has two major areas of activity, namely, documentation and research. The correlation of data and the publication of tables is one of the aims of the research program. The research staff in 1959 consisted of the Director, Y. S. Touloukian, and six full- or part-time professional people. The overall program has been supported to date primarily by industrial firms. TPRC is now receiving substantial support for its complilation program from the Wright Air Development Division, Air Research and Development Command.

<u>Substances</u>: In its documentation activities TPRC collects information on <u>all</u> classes of materials. The preparation of data tables is undertaken on a priority basis by selecting properties and materials of current interest.

<u>Properties:</u> The initial effort is confined to seven properties, namely: thermal conductivity; viscosity; thermal emissivity, absorptivity and reflectivity; diffusion coefficient; specific heat; thermal diffusivity; and Prandtl number.

Sources of Data: World literature; foreign and English language abstracting services; governmental, academic, and industrial research reports; Master's and Doctoral theses from accredited colleges and universities; and cooperative arrangements with major research laboratories in the U. S. and abroad.

Criticality: The stated aim is to produce, whenever possible, an internally consistent set of "most probable values" of a particular property and material and to supplement available experimental data by semi-empirical and theoretical methods. The first table projects have been on the thermal conductivity of metals and alloys and the thermal conductivity and viscosity of gases and vapors. In the case of engineering alloys, the inability to identify a particular material uniquely at times makes the selection of a single best value impossible. The tables of recommended values for gases are accompanied by departure plots.

Use of Nomenclature, Symbols, Units, Physical Constants: Policies concerning symbols, units, etc. will take into account the dual orientation to engineering and pure science.

Currency: The aim is to achieve coverage on a current basis.

Format: The pre-publication form is an 11" x 17" sheet printed on one side. The experimentally determined data for each material are presented in graphical form. A table of experimental conditions and a table of data accompany each graph. Each material studied is assigned a serial number, and all figures and tables pertaining to that material bear the assigned number. Literature references are given at the end of the data set. When there is sufficient material for formal publication, there will be a division into three volumes. Volume I will cover metals and alloys; Volume II, gases and liquids; and Volume III, non-metallic solids. Division of a volume into chapters will be according to property.

<u>Publication and Distribution:</u> Pre-publication data sheets are distributed to all sponsors and a number of cooperating institutions as soon

as they are available. When a sufficient number of sheets has accumulated, they will be published formally for broad distribution. To date, sheets have been prepared on the thermal conductivity of 33 metals and 9 binary alloys and on the thermal conductivity and viscosity of 15 gases.

Comment: To date, TPRC has placed greater emphasis on literature search methods and documentation techniques. The first tangible product of this activity is the forthcoming three-book volume, "Retrieval Guide to Thermophysical Properties Research Literature," Volume I, 1960. The laboratory research program and data evaluation projects are being accelerated gradually.

V. SPECTROSCOPIC PROJECTS

V-A. Atomic Spectra

V-A-1. Atomic Energy Levels (and an Ultraviolet Multiplet Table)

Organization: This project was established at the National Bureau of Standards in 1946 with the encouragement of the National Research Council Committee on Line Spectra of the Elements. The project is under the supervision of Charlotte E. Moore of the Spectroscopy Section of the Atomic and Radiation Physics Division. Outside experts, in the U. S. and abroad, help by making calculations and supplying unpublished research results. NBS supplies technical, editorial, library, and secretarial help.

<u>Substances:</u> In so far as possible, all the elements are to be covered.

<u>Properties:</u> Atomic energy levels are presented as completely as possible. Hyperfine structure ascribed to atomic nuclei is not covered. Selected ultraviolet multiplets are published.

Sources of Data: Mainly open literature and unpublished results. In 1914 William F. Meggers of NBS started a comprehensive card catalog of data and references which has been carefully kept up to date.

<u>Criticality</u>: The highly competent staff appraises the literature with discrimination. The many outside collaborators are recognized experts.

Use of Nomenclature, Symbols, Units, Physical Constants: The terminology and constants used are those acceptable to experts in the field. A special effort has been made to introduce a uniform scheme of spectroscopic notation.

<u>Currency</u>: The elements are being treated systematically in the order of their atomic numbers. Each new volume contains a section "Additions and Corrections" to earlier volumes. The card catalog of data and references is kept current at all times.

Format: ATOMIC ENERGY LEVELS is published in book form. The tabular form of presentation resulted from a census of the opinions of experts. The spectra are indexed and arranged in the order of their increasing atomic number. References are given for each spectrum. Also listed are references covering the complete analysis, classified lines, energy or Grotian diagrams, and Zeeman data. AN ULTRAVIOLET MULTIPLET TABLE is in booklet form. Data are presented in tables, the elements being treated in order of increasing atomic number. References precede each table.

Publication and Distribution: ATOMIC ENERGY LEVELS is published as NBS Circular 467. Volumes I, II, and III appeared between 1949 and 1958; they contain the data for elements hydrogen through lanthanum (at. no. 57) and hafnium through actinium (72 through 89). Demand for Volume I has been great enough to require reprintings in 1950, 1954 and 1960. Volume IV will deal with the two groups of "rare earth" spectra. The complexity of the remaining spectra and the large amount of new data to be determined make Volume IV a formidable undertaking that may well take 8 to 10 years for completion. AN ULTRAVIOLET MULTIPLET TABLE is published in sections as NBS Circular 488. Sections 1 and 2, which parallel Volumes I and II of ATOMIC ENERGY LEVELS, appeared in 1950 and 1952, respectively. Both sections were reprinted in 1956. Section 3 is in preparation. There will be also a Finding List of the wave lengths in all sections of the Multiplet Table. Volumes I-III of ATOMIC ENERGY LEVELS and Sections 1 and 2 of AN ULTRAVIOLET MUL-TIPLET TABLE are available from the Superintendent of Documents, U. S. Government Printing Office, Washington 25, D. C. Prices are given below.

Atomic Energy Levels as Derived from The Analyses of Optical Spectra

by Charlotte E. Moore

Volume I, The Spectra of Hydrogen, Deuterium, Tritium, Helium, Lithium, Beryllium, Boron, Carbon, Nitrogen, Oxygen, Fluorine, Neon, Sodium, Magnesium, Aluminum, Silicon, Phosphorus, Sulfur, Chlorine, Argon, Potassium, Calcium, Scandium, Titanium, and Vanadium; 1949; xliii + 309 pp.; \$4.75.

Volume II, The Spectra of Chromium, Manganese, Iron, Cobalt, Nickel, Copper, Zinc, Gallium, Germanium, Arsenic, Selenium, Bromine, Krypton, Rubidium, Strontium, Yttrium, Zirconium, and Niobium; 1952; xxxi + 227 pp.; \$4.00.

Volume III, The Spectra of Molybdenum, Technetium, Ruthenium, Rhodium, Palladium, Silver, Cadmium, Indium, Tin, Antimony, Tellurium, Iodine, Xenon, Cesium, Barium, Lanthanum--Hafnium, Tantalum, Tungsten, Rhenium, Osmium, Iridium, Platinum, Gold, Mercury, Thallium, Lead, Bismuth, Polonium, Radon, Radium, and Actinium; 1958; xxxviii + 245 pp.; \$2.50.

An Ultraviolet Multiplet Table

by Charlotte E. Moore

Section 1, The Spectra of Hydrogen, Helium, Lithium, Beryllium, Boron, Carbon, Nitrogen, Oxygen, Fluorine, Neon, Sodium, Magnesium, Aluminum, Silicon, Phosphorus, Sulfur, Chlorine, Argon, Potassium, Calcium, Scandium, Titanium, and Vanadium; 1950; vii + 78 pp.; 55 cents.

Section 2, The Spectra of Chromium, Manganese, Iron, Cobalt, Nickel, Copper, Zinc, Gallium, Germanium, Arsenic, Selenium, Bromine, Krypton, Rubidium, Strontium, Yttrium, Zirconium, and Niobium; 1952; v + 115 pp.; 70 cents.

Note: Although not part of this project another publication by Charlotte Moore of great current importance has recently been reprinted by NBS. This is a MULTIPLET TABLE OF ASTROPHYSICAL INTEREST (Contributions from the Princeton University Observatory No. 20, Revised Edition) originally published in 1945. It bears the designation NBS Technical Note No. 36, 1960 (PB 151395) and is available for \$4.00 from the Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C.

V-B. Infrared Spectra

V-B-1. American Petroleum Institute Research Project 44

Organization: (See I-1.) APIRP 44 began publishing infrared spectral data in 1943. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

<u>Substances</u>: Mostly hydrocarbons and related compounds; a few other compounds of interest to the petroleum industry.

<u>Properties:</u> Infrared absorption spectra. [APIRP 44 also publishes physical and thermodynamic data (see I-1) and several other types of spectra (see V-C-1, V-D-1, V-E-1, and V-F-1).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra are removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds result in a continual improvement in the quality of the catalog.

<u>Units:</u> Percent transmittance is plotted against both wave length in microns and frequency in cm⁻¹.

Currency: Revisions and additions are issued at regular intervals.

Format: The form of publication is the loose-leaf sheet. Sheets dated before June 30, 1959, are $8" \times 10 \ 1/2"$; those after are $8 \ 1/2" \times 11"$. Spectral curves are on one side of a sheet, and frequently a table of wave lengths, absorptivities, or related quantities is given on the reverse side. Sheets are arranged in order of serial number which is the order of inclusion in the catalog. There is a compound index arranged by compound type and a numerical index arranged in order of increasing serial number. The name of the contributing laboratory is given on the spectral sheet and identified in the indexes by a code letter or letters.

Publication and Distribution: Covering title of the loose-leaf sheets is INFRARED SPECTRAL DATA. The total number of valid infrared spectra in the catalog as of June 30, 1960, was 2119. New sheets are distributed semiannually by the Agricultural and Mechanical College of Texas, Department of Chemistry, College Station, Texas. Distribution of the sheets is made to three categories of recipients (see I-1). The sheets are sold, in complete sets only, at 10 cents per sheet. As of June 30, 1960, the total number of valid sheets, was 2240.

V-B-2. Analytical Applications of Far Infrared Spectra

Organization: This project is carried out at the Wright Air Development Division, Wright-Patterson Air Force Base, Ohio. It is sponsored and financed by the Air Research and Development Command, United States Air Force. Leo F. Salzberg, Chief, Physics Laboratory, directs the project. A working staff makes measurements in the Materials Central of WADD under the immediate supervision of Freeman F. Bentley.

<u>Substances:</u> Aliphatic and aromatic hydrocarbons, bromohydrocarbons.

Properties: Infrared absorption spectra in the 15 to 35 micron range.

Sources of Data: Spectra recorded on a modified Perkin Elmer Model 21 Spectrophotometer in the Materials Laboratory.

Criticality: The spectra are reviewed by a staff of spectroscopists.

<u>Units:</u> Percent transmittance is plotted against both wave length in microns and frequency in cm⁻¹.

Format: Spectral curves and tables in technical reports.

Publication and Distribution: The spectra of this project have been published in WADC Technical Reports 57-359, 57-413, 58-198, and Supplement 1 to 58-198. The first of these is no longer available, but the last three may be obtained from the Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C. The order numbers and prices are PB 131403, \$1.00; PB 151677, \$1.50; and PB 151677 S, 50 cents.

V-B-3. The Anderson Physical Laboratory Near Infrared Spectra

Organization: The Anderson Physical Laboratory, of which Scott Anderson is founder and director, is located at 609 South Sixth St., Champaign, Ill. This laboratory, which does industrial research, analytical services, and consulting, started issuing near infrared data in 1958. The spectra are measured under the supervision of Anderson Laboratory personnel.

Substances: Mostly organic, some inorganic compounds.

<u>Properties:</u> Infrared absorption spectra in the 0.7 to 3.2 micron range.

Sources of Data: Spectra measured in the Anderson Laboratory on a Beckman DK-2 ratio recording spectrophotometer.

<u>Criticality</u>: Spectra are reviewed by a panel of experienced spectroscopists.

<u>Units:</u> Percent transmittance is plotted against wave length in microns.

Format: Two different spectra are presented on one side of an 8 1/2" x 11" loose-leaf sheet. Each curve is numbered, and the conditions of measurement are listed beside the curve. Alphabetical and formula indexes are made twice yearly.

<u>Publication and Distribution:</u> This group will soon discontinue publishing new curves. However, a total of 1200 ANDERSON NEAR INFRARED SPECTRA and about 500 spectra of polynuclear compounds will be available by purchase directly from the Anderson Physical Laboratory.

V-B-4. Le Centre d'Information de l'Infra-rouge (C.I.R.)

Organization: The C. I.R. was established in 1956 by Le Groupement pour l'Avancement des Méthodes Spectrographiques (G. A. M. S.) to coordinate the collection of infrared absorption spectra from international sources. Communications should be directed c/o E. Loeuille, G. A. M. S., L. N. E., 1 rue Gaston-Boissier, Paris-XV^e, France. Cooperating groups include Ministère de la Défense Nationale et des Forces Armées and industrial and educational institutions.

Substances: Organic and inorganic compounds.

Properties: Infrared absorption spectra.

Sources of Data: The Sadtler, DMS, APIRP 44, and Coblentz collections and the following French sources: Institut Français de Pétrole, R. N. U. Renault, Rhone-Poulenc, St. Gobain, and individual members of G. A. M. S.

<u>Criticality</u>: Spectra are reviewed by a staff of spectroscopists before standard spectrograms are issued.

<u>Units:</u> Percent transmittance is plotted against both wave length in microns and frequency in cm⁻¹.

<u>Format:</u> A spectral curve and a table of absorption bands for one compound appear on one side of a loose-leaf sheet, $9 \frac{1}{2}$ " x 17". Additional information and the data source are given at the side.

Publication and Distribution: C. I. R. has published about 200 spectra. These have been distributed to various cooperating groups. The publication of spectra is being discontinued but may be resumed if circumstances permit.

V-B-5. Coblentz Society Committee on Infrared Absorption Spectra

Organization: This committee of seven was established in 1957 by the Coblentz Society to expedite the production and distribution of standard reference spectra. Chairman of the committee is Clara D. Smith, 920 Bayard Park Drive, Evansville 13, Ind. Spectra are reviewed by ten regional collectors. Arrangements have been made with the Sadtler Research Laboratories (see V-B-9) for publishing these spectra in their Midget Edition. A financial return to the Society from the sale of the spectra supports the program.

Substances: Pure compounds and commercial products.

Properties: Infrared absorption spectra in the 2 to 30 micron range.

Sources of Data: Spectra submitted by investigators.

<u>Criticality</u>: Different spectra for the same substance are forwarded to a central committee for editing and cross-comparison to insure that the best spectra are published. The long-range goal is a collection of high-resolution, accurate spectra of very pure compounds.

Nomenclature: Submitted spectra are checked for completeness and consistency of compound or material name.

Format: The collected spectra are published three curves to an $8\ 1/2" \times 11"$ page (Sadtler's Midget Edition). Superimposed on each spectrum is the following information: compound name; empirical or structural formula; values of other properties, e. g., boiling point; source of information.

Publication and Distribution: The Coblentz Society copyrights the spectra, but participating publishers may receive authorization to use them. Orders for the COBLENTZ SOCIETY SPECTRA may be sent to The Sadtler Research Laboratories, 1517 Vine Street, Philadelphia 2, Pa. The price is \$100.00 per 1000 spectra. A completed set of 1000 spectra was available by mid-1960.

V-B-6. Documentation of Molecular Spectroscopy (DMS)

Organization: Documentation of Molecular Spectroscopy is a card system published jointly by Butterworths Scientific Publications, 88 Kingsway, London, W.C. 2, England, and Verlag Chemie GmbH, Weinheim/Bergstrasse, West Germany. The data are prepared by well-qualified experts working under the direction of British and German

groups. The former is headed by H. W. Thompson, Oxford University, and the latter by H. Kaiser, Institut für Spektrochemie, Dortmund. DMS started publication in 1956.

Substances: Organic compounds now, inorganic later.

Properties: Infrared absorption spectra.

Sources of Data: Current literature; collections from industrial and academic laboratories in Europe, the U. S. A., and Canada.

Criticality: Data are evaluated by an advisory committee.

<u>Units:</u> Percent absorption and percent transmittance are plotted against frequency in cm⁻¹ and wave length in microns.

Format: DMS issues two kinds of Keysort (4 3/4" x 8 1/4") cards: (1) literature cards, yellow, giving abstracts of important articles on spectroscopic problems or containing useful spectra; (2) spectral cards, rose-colored, of which there are two types, (A) those for the infrared spectra of organic compounds and (B) those for the infrared spectra of technical products, mixtures, and polymers and natural substances of undetermined constitution. The front side of a spectral card gives the name, main physical properties, molecular and structural formulas of the compound, the author or source of the spectrum, and the conditions under which the spectrum was measured. The reverse side shows the spectrum and a table of frequencies of the chief bands and their approximate intensities. Identical English and German editions are issued. The cards are coded by punching the edges in the following way. The upper and right-hand sides are used to code the structural features of the compound, and the bottom and left-hand sides to mark the positions of the main bands.

Publication and Distribution: Subscribers to the DMS card service receive about 2000 cards a year in batches of 500 at intervals of about three months. The spectral cards make up about 80% of those issued. Each subscriber is provided with a complete "Instruction and Coding Manual." Exclusive U. S. agent for the English edition is Spex Industries, Inc., 205-02 Jamaica Ave., Hollis 23, N. Y. Cost of an annual subscription is \$182.00.

V-B-7. Manufacturing Chemists Association Research Project on Properties of Chemical Compounds

Organization: (See I-4.) The spectroscopic program of MCA began in 1959. Cooperating in the collection of spectral data are numerous

industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

Substances: Non-hydrocarbon chemical compounds.

<u>Properties:</u> Infrared absorption spectra. [MCA also publishes physical and thermodynamic data (see I-4) and several other types of spectra (see V-C-2, V-D-2, V-E-2, and V-F-2).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra will be removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds will result in a continual improvement in the quality of the catalog.

<u>Currency:</u> Revisions and additions will be issued at regular intervals.

<u>Format</u>: This catalog is complementary to the API catalog of infrared spectra, using the same standard form with similar indices (see V-B-1).

Publication and Distribution: Covering title of the loose-leaf sheets is INFRARED SPECTRAL DATA: The total number of valid infrared spectra in the catalog as of June 30, 1960, was 108. New sheets are distributed semiannually by the Manufacturing Chemists Association, 1825 Connecticut Ave., N. W., Washington, D. C. Distribution of the sheets is made to three categories of recipients (see I-4).

V-B-8. National Research Council Committee on Spectral Absorption Data

Organization: The NRC Committee on Spectral Absorption Data is a joint committee of the Division of Physical Sciences and the Division of Chemistry and Chemical Technology. Chairman of the fifteen-man committee is Wallace R. Brode. John J. Comeford, who is the committee secretary, heads a small staff at the National Bureau of Standards, Washington, D. C. NBS provides working space and the equivalent of one and a half employees. Otherwise the project is supported by the sale of its publications. The group has been publishing data continuously since 1952.

Substances: Mostly organic compounds, a few inorganic.

Properties: Infrared absorption spectra.

Sources of Data: Contributions from spectroscopists, measurements made at NBS, selected English-language journals.

<u>Criticality:</u> When possible there is comparison of different spectra for the same compound before publication. The emphasis is on quality rather than quantity.

<u>Units:</u> Percent transmittance is plotted against both wave length in microns and frequency in cm⁻¹.

<u>Currency</u>: Output in the past has been considerably less than that of some of the commercial groups but has recently increased three-fold.

Format: Two forms of publication are used, a 6 1/2" x 7 1/2" edge-punch card and an 8 1/2" x 11" sheet. The following information is coded and punched on the COMPOUND CARDS: position of major absorption bands, melting or boiling point, molecular functional groups, and number of carbon atoms. The body of the card contains general information about the compound, information about the particular sample of the compound for which a spectrum is given, and a table that lists literature references and indicates the type of data found in each article. The reverse side of the card contains the spectrum for the particular compound sample and information that characterizes the sample and describes the conditions of measurement. The COMPOUND SHEETS bear the same information appearing on the cards. The committee also prepares and distributes BIBLIOGRAPHY CARDS and BIBLIOGRAPHY SHEETS which give abstracts of papers on infrared spectroscopy, instrumentation, and related subjects.

Publication and Distribution: As of January 1, 1960, there were 2015 Compound Cards (on 1728 compounds) and 1050 Bibliography Cards. Current output is about 800 Compound Cards per year. COMPOUND CARDS (or sheets) are sold on a subscription basis only for 10 cents each. BIBLIOGRAPHY CARDS (or sheets) are sold on a subscription basis only for five cents each. Orders should be placed with the National Research Council Committee on Spectral Absorption Data, Room 202, Chemistry Building, National Bureau of Standards, Washington 25, D.C. There is a possibility that publication of compound and bibliography cards and sheets will be terminated in December 1960. Publication of a circular containing the bibliographic and spectral data in the master file is under consideration.

V-B-9. The Sadtler Research Laboratories

Organization: Samuel P. Sadtler & Son, Inc., an industrial research laboratory which has been issuing spectra continuously since 1947, is located at 1517 Vine St., Philadelphia 2, Pa. Philip Sadtler is President and Director of Research. Other Sadtler services include sponsored industrial research and spectral analyses.

<u>Substances:</u> Organic compounds (most recently including steroids) and commercial products.

<u>Properties:</u> Infrared spectra have been issued since 1947; coverage has recently been extended to include near infrared. (Sadtler has also recently started to issue ultraviolet spectra. See IV-C-3).

Sources of Data: Spectra determined in the Sadtler laboratories on compounds contributed by industrial and research organizations and educational institutions.

<u>Criticality</u>: Each spectrum measured in the Sadtler laboratories is checked three times and then sent to an outside laboratory for an additional check. The quality of an individual spectrum depends in part on the purity of the contributed compound. Sadtler invites users of the SADTLER STANDARD SPECTRA to send in results of measurements made on different preparations of the same compounds in the Standard Spectra catalog; lists of verified spectra are then sent to subscribers.

<u>Units:</u> Percent transmittance is plotted against both wave length in microns and frequency in cm⁻¹.

<u>Currency:</u> Regular publication policy adds many new spectra annually.

Format: SADTLER STANDARD SPECTRA, a collection of infrared spectrograms of organic compounds that is used for the identification of unknown spectra, is published in two forms: (1) Regular Edition (cards, 5" x 13") and (2) Midget Edition (3 spectra on an 8 1/2" x 11" page). Spectra are located by the use of one of five INDICES or the SADTLER SPEC-FINDER (a book method of locating infrared spectra by the bands). SADTLER COMMERCIAL SPECTRA, a collection of infrared spectrograms of several thousand commercial preparations that do not meet the purity requirements of the standard spectra compounds, is published separately. For the SADTLER NEAR INFRARED SPECTRA, two, three, or four cell thicknesses or concentrations are scanned for each substance; the spectrum of each concentration or thickness is printed separately, two on an 8 1/2" x 11" page. The indices now used for the Standard Spectra will

also be applicable to the Near Infrared Spectra, but a special numerical index will also be necessary. A NEAR INFRARED NUMERICAL INDEX is to be published. SADTLER STEROID SPECTRA is published as a separate book. By special arrangement with the Coblentz Society, Sadtler also publishes as a separate book the COBLENTZ SOCIETY SPECTRA (see V-B-5).

Publication and Distribution: The complete standard spectra catalog through 1960 comprises 17,350 spectra. The regular edition (cards) of SADTLER STANDARD SPECTRA may be purchased singly, in groups, or in complete sets; the midget edition is sold only in designated units. Purchase price of all spectra issued through 1960 is \$4,370.00 for the regular edition and \$1,790.00 for the midget edition. SADTLER COMMERCIAL SPECTRA are 50 cents each but must be purchased in complete designated units; special rates are available to standard spectra subscribers. By January 1960, 1000 NEAR INFRARED SPECTRA were available; these are \$250.00 per 1000 spectra. SADTLER STEROID SPECTRA and the COBLENTZ SOCIETY SPECTRA may be purchased separately, the former for \$100.00 per 1000 spectra and the latter for \$1,200.00 per 1500 spectra. Beginning in 1961, 2000 standard spectra, 1000 near infrared spectra and 4000 commercial spectra will be published yearly.

V-C. Electronic Spectra

V-C-1. American Petroleum Institute Research Project 44

Organization: (See I-1.) APIRP 44 began publishing ultraviolet spectral data in 1945. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

<u>Substances</u>: Mostly hydrocarbons and related compounds; a few other compounds of interest to the petroleum industry.

<u>Properties:</u> Ultraviolet absorption spectra. [APIRP 44 also publishes physical and thermodynamic data (see I-1) and several other types of spectra (see V-B-1, V-D-1, and V-F-1).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra are removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds result in a continual improvement in the quality of the catalog.

<u>Units:</u> Absorbance is plotted against both wave length in Angstrom units and frequency in cm⁻¹.

Currency: Revisions and additions are issued at regular intervals.

Format: The form of publication is the loose-leaf sheet. Sheets dated before June 30, 1959, are 8" x 10 1/2"; those after are 8 1/2" x 11". Spectral curves are on one side of a sheet, and frequently a table of wave lengths, slit widths, optical densities (or absorbances) is given on the reverse side. Sheets are arranged in order of serial number which is the order of inclusion in the catalog. There is a compound index arranged by compound type and a numerical index arranged in order of increasing serial number. The name of the contributing laboratory is given on the spectral sheet and identified in the indexes by a code letter or letters.

Publication and Distribution: Covering title of the loose-leaf sheets is ULTRAVIOLET SPECTRAL DATA. The total number of valid ultraviolet spectra in the catalog as of June 30, 1960, was 806. New sheets are distributed semiannually by the Agricultural and Mechanical College of Texas, Department of Chemistry, College Station, Texas. Distribution of the sheets is made to three categories of recipients (see I-1). The sheets are sold, in complete sets only, at 10 cents per sheet. As of June 30, 1960, the total number of valid sheets, including index sheets, was 845.

V-C-2. Manufacturing Chemists Association Research Project on Properties of Chemical Compounds

Organization: (See I-4.) The spectroscopic program of MCA began in 1959. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

Substances: Non-hydrocarbon chemical compounds.

<u>Properties:</u> Ultraviolet absorption spectra. [MCA also publishes physical and thermodynamic data (see I-4) and several other types of spectra (see V-B-7, V-D-2, V-E-2, and V-F-2).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra will be removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds will result in a continual improvement in the quality of the catalog.

<u>Currency</u>: Revisions and additions will be issued at regular intervals.

Format: This catalog is complementary to the API catalog of ultraviolet spectra, using the same standard form with similar indices (see V-C-1).

Publication and Distribution: Covering title of the loose-leaf sheets is ULTRAVIOLET SPECTRAL DATA. The total number of valid ultraviolet spectra in the catalog as of June 30, 1960, was 13. New sheets are distributed semiannually by the Manufacturing Chemists Association, 1825 Connecticut Ave., N.W., Washington, D. C. Distribution of the sheets is made to three categories of recipients (see I-4). Sheets are available on a subscription basis for 10 cents each. As of June 30, 1960, the total number of valid sheets, including index sheets, was 18.

V-C-3. Organic Electronic Spectral Data, Inc.

Organization: O.E.S.D.I. is a non-profit group that owes its existence to an informal meeting in 1956 of physical-organic chemists who were concerned about the state of ultraviolet literature. The group was incorporated and the first officers were elected in 1957. Information about O.E.S.D.I. may be obtained from either of the two original co-editors, Mortimer J. Kamlet, U.S. Naval Ordnance Laboratory, Silver Spring, Md., or Herbert E. Ungnade, Los Alamos Scientific Laboratory, Los Alamos, N. M. More than fifty chemists from government, industry, and universities did the literature searching and abstracting for the first two volumes on a volunteer basis. Original financial support came in the form of an advance from the publisher. Later support came from instrument manufacturers and other groups. Card processing was carried out in Jerusalem, Israel, by graduate students of the Hebrew University under a grant from the National Science Foundation. Continuity on a volunteer basis is planned.

Substances: All in literature covered.

Properties: Ultraviolet and visible spectra.

Sources of Data: World literature.

<u>Criticality</u>: The quality of the data varies since all in the literature are compiled. An effort has been made to eliminate obvious errors.

Use of Nomenclature, Symbols, Units, Physical Constants: Chemical Abstracts nomenclature has been used. Considerable effort has gone into converting all the data into the same units. The units used are those recommended by the Joint Committee on Nomenclature in Applied Spectroscopy (Society for Applied Spectroscopy and Committee E-2 of the American Society for Testing Materials). O. E. S. D. I. has made recommendations on the use of preferred units for wave length and absorption intensity to the Commission on Molecular Spectroscopy of the International Union of Pure and Applied Chemistry.

<u>Currency</u>: Volumes I and II, covering the years 1946 through 1955, were available in early 1961. Volume III, covering 1956-1957, is now in preparation; abstracting for Volume IV, covering 1958-1959, is almost complete. Eventually there will be annual supplements.

<u>Format:</u> Tables giving empirical formula, name, solvent (or phase), wave lengths of all maxima, molar absorptivities, and literature reference are published in book form. Compounds are arranged according to molecular formula.

Publication and Distribution: ORGANIC ELECTRONIC SPECTRAL DATA is published by Interscience Publishers, Inc., 250 Fifth Avenue, New York 1, N. Y. Volume I costs \$28.50 and Volume II, \$17.50. Slightly lower prices are available on a subscription basis.

V-C-4. The Sadtler Research Laboratories

Organization: (See V-B-9.) The date of publication of the first group of ultraviolet spectra was September 1, 1959.

Substances: Organic compounds.

<u>Properties:</u> Ultraviolet absorption spectra from 210 to 350 millimicrons. [Sadtler also publishes infrared spectra (see V-B-9).]

Sources of Data: Spectra determined in the Sadtler laboratories on compounds contributed by industrial and research organizations and educational institutions.

<u>Criticality</u>: Each spectrum measured in the Sadtler laboratories is checked three times and then sent to an outside laboratory for an additional check. The quality of an individual spectrum depends in part on the purity of the contributed compound. Sadtler advertising literature states only that samples at least 98 percent pure are used. No criteria of purity are presented.

Nomenclature and Units: Chemical Abstracts names are used. Absorbance is plotted against wave length in millimicrons.

<u>Currency:</u> Regular publication policy adds many new spectra annually.

Format: SADTLER U-V SPECTRA are printed one to an 8 1/2" x 11" page. The indices now used for the Standard (Infrared) Spectra will be applicable to the U-V Spectra, but a special numerical index will also be necessary. An ULTRAVIOLET NUMERICAL INDEX is to be published.

<u>Publication and Distribution:</u> As of September 1960, 1000 ultraviolet spectra were available by subscription. Beginning in 1961, 2000 spectra will be published annually. Purchase price of \$200.00 per 1000 spectra includes the cost of indexes and binders.

V-D. Mass Spectra

V-D-1. American Petroleum Institute Research Project 44

Organization: (See I-1.) APIRP 44 began publishing mass spectral data in 1947. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

<u>Substances:</u> Mostly hydrocarbons and related compounds; a few other compounds of interest to the petroleum industry.

<u>Properties:</u> Mass spectra. [APIRP 44 also publishes physical and thermodynamic data (see I-1) and several other types of spectra (see V-B-1, V-C-1, V-E-1, and V-F-1).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality:</u> The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra are removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds result in a continual improvement in the quality of the catalog.

Currency: Revisions and additions are issued at regular intervals.

Format: The form of publication is the loose-leaf sheet. Sheets dated before June 30, 1959, are $8'' \times 10 \ 1/2''$; those after are $8 \ 1/2'' \times 11''$. Data are tabulated on one side of a sheet. Sheets are arranged in order of serial number which is the order of inclusion in the catalog. There is a compound index arranged by compound type and a numerical index arranged in order of increasing serial number. The name of the

contributing laboratory is given on the spectral sheet and identified in the indexes by a code letter or letters.

Publication and Distribution: Covering title of the loose-leaf sheets is MASS SPECTRAL DATA. The total number of valid mass spectra in the catalog as of June 30, 1960, was 1752. New sheets are distributed semiannually by the Agricultural and Mechanical College of Texas, Department of Chemistry, College Station, Texas. Distribution of the sheets is made to three categories of recipients (see I-1). The sheets are sold, in complete sets only, at 10 cents per sheet. As of June 30, 1960, the total number of valid sheets, including index sheets, was 1845.

V-D-2. Manufacturing Chemists Association Research Project on Properties of Chemical Compounds

Organization: (See I-4.) The spectroscopic program of MCA began in 1959. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

Substances: Non-hydrocarbon chemical compounds.

Properties: Mass spectra. [MCA also publishes physical and thermodynamic data (see I-4) and several other types of spectra (see V-B-7, V-C-2, V-E-2, and V-F-2).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra will be removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds will result in a continual improvement in the quality of the catalog.

<u>Currency</u>: Revisions and additions will be issued at regular intervals.

Format: This catalog is complementary to the API catalog of mass spectra, using the same standard form with similar indices (see V-D-1).

Publication and Distribution: Covering title of the loose-leaf sheets is MASS SPECTRAL DATA. The total number of valid mass spectra in the catalog as of June 30, 1960, was 114. New sheets are distributed semiannually by the Manufacturing Chemists Association, 1825 Connecticut Ave., N.W., Washington, D. C. Distribution of the sheets is

made to three categories of recipients (see I-4). Sheets are available on a subscription basis for 10 cents each. As of June 30, 1960, the total number of valid sheets, including index sheets, was 120 (estimated).

V-E. Raman Spectra

V-E-1. American Petroleum Institute Research Project 44

Organization: (See I-1.) APIRP 44 began publishing Raman spectral data in 1948. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

<u>Substances:</u> Mostly hydrocarbons and related compounds; a few other compounds of interest to the petroleum industry.

<u>Properties:</u> Raman spectra. [APIRP 44 also publishes physical and thermodynamic data (see I-1) and several other types of spectra (see V-B-1, V-C-1, V-D-1, and V-F-1).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra are removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds result in a continual improvement in the quality of the catalog.

Currency: Revisions and additions are issued at regular intervals.

Format: The form of publication is the loose-leaf sheet. Sheets dated before June 30, 1959, are 8" x 10 1/2"; those after are 8 1/2" x 11". Data are presented graphically on one side of a sheet and in tables on the reverse side. Sheets are arranged in order of serial number which is the order of inclusion in the catalog. There is a compound index arranged by compound type and a numerical index arranged in order of increasing serial number. The name of the contributing laboratory is given on the spectral sheet and identified in the indexes by a code letter or letters.

Publication and Distribution: Covering title of the loose-leaf sheets is RAMAN SPECTRAL DATA. The total number of valid Raman spectra in the catalog as of June 30, 1960, was 363. (The advent of automatic, photoelectric Raman instrumentation will now make it possible to enlarge the Raman Catalog at a faster rate.) New sheets are distributed semiannually by the Agricultural and Mechanical College of

Texas, Department of Chemistry, College Station, Texas. Distribution of the sheets is made to three categories of recipients (see I-1). The sheets are sold, in complete sets only, at 10 cents per sheet. As of June 30, 1960, the total number of valid sheets, including index sheets, was 393.

V-E-2. Manufacturing Chemists Association Research Project on Properties of Chemical Compounds

Organization: (See I-4.) The spectroscopic program of MCA began in 1959. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

Substances: Non-hydrocarbon chemical compounds.

<u>Properties:</u> Raman spectra. [MCA also publishes physical and thermodynamic data (see I-4) and several other types of spectra (see V-B-7, V-C-2, V-D-2, and V-F-2).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality:</u> The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra will be removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds will result in a continual improvement in the quality of the catalog.

<u>Currency</u>: Revisions and additions will be issued at regular intervals.

Format: This catalog is complementary to the API catalog of Raman spectra, using the same standard form with similar indices (see V-E-1).

<u>Publication and Distribution</u>: The total number of valid Raman spectra in the catalog as of December 31, 1960, was about 100. Sheets are distributed semiannually by the Manufacturing Chemists Association, 1825 Connecticut Ave., N.W., Washington, D. C. Distribution of the sheets is made to three categories of recipients (see I-4).

V-F. Nuclear Magnetic Resonance Spectra

V-F-1. American Petroleum Institute Research Project 44

Organization: (See I-1.) APIRP 44 began publishing nuclear magnetic resonance spectral data in 1959. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

<u>Substances:</u> Mostly hydrocarbons and related compounds; a few other compounds of interest to the petroleum industry.

<u>Properties:</u> Nuclear magnetic resonance spectra. Proton magnetic resonance is the first type to be covered; it is hoped that other nuclei can be included soon. [APIRP 44 also publishes physical and thermodynamic data (see I-1) and several other types of spectra (see V-B-1, V-C-1, V-D-1, and V-E-1).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra are removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds will result in a continual improvement in the quality of the catalog.

Currency: Revisions and additions are issued at regular intervals.

Format: The form of publication is the loose-leaf sheet (8 1/2" x 11"). The spectral curve and information about the compound studied, the instrument used, and the conditions of measurement appear on one side of the sheet. Sheets are arranged in order of serial number which is the order of inclusion in the catalog. The name of the contributing laboratory is given on the spectral sheet.

Publication and Distribution: Covering title of the loose-leaf sheets is NUCLEAR MAGNETIC RESONANCE SPECTRAL DATA. The total number of valid nuclear magnetic resonance spectra in the catalog as of June 30, 1960, was eight. New sheets are distributed semiannually by the Agricultural and Mechanical College of Texas, Department of Chemistry, College Station, Texas. Distribution of the sheets is made to three categories of recipients (see I-1). The sheets are sold, in complete sets only, at 10 cents per sheet. As of June 30, 1960, the total number of valid sheets, including index sheets, was 13.

V-F-2. Manufacturing Chemists Association Research Project on Properties of Chemical Compounds

Organization: (See I-4.) The spectroscopic program of MCA began in 1959. Cooperating in the collection of spectral data are numerous industrial, academic, and governmental laboratories. Alfred Danti, the Assistant Director, is in charge of the spectral data program.

Substances: Non-hydrocarbon chemical compounds.

Properties: Nuclear magnetic resonance spectra. [MCA also publishes physical and thermodynamic data (see I-4) and several other types of spectra (see V-B-7, V-C-2, V-D-2, and V-E-2).]

Sources of Data: Spectra measured in cooperating laboratories.

<u>Criticality</u>: The project staff selects spectra from those submitted by contributing laboratories. Inferior spectra will be removed from the catalog as better ones become available. The constantly improving instrumentation and increasing availability of pure compounds will result in a continual improvement in the quality of the catalog.

<u>Currency</u>: Revisions and additions will be issued at regular intervals.

<u>Format:</u> This catalog is complementary to the API catalog of nuclear magnetic resonance spectra, using the same standard form with similar indices (see V-F-1).

Publication and Distribution: The total number of valid nuclear magnetic resonance spectra in the catalog as of December 31, 1960, was about 50. Sheets are distributed semiannually by the Manufacturing Chemists Association, 1825 Connecticut Ave., N.W., Washington, D.C. Distribution of the sheets is made to three categories of recipients (see I-4).

V-G. Spectral Indexing System

V-G-1. American Society for Testing Materials Committee on Absorption Spectroscopy

Organization: ASTM does not publish any spectra, but it does provide indexing systems for the fields of absorption spectrophotometry. This indexing service is the outgrowth of one of the aims of ASTM Committee E-13 on Absorption Spectroscopy, the exchange of information in the fields of spectroscopy. The ASTM indexing systems facilitate the sorting of spectral data for matching spectrograms in qualitative analysis

and for correlating chemical structure and absorption band positions. The indexes are based on the Wyandotte systems developed at Wyandotte Chemical Corporation by L. E. Kuentzel in cooperation with Committee E-13. Spectra are coded by volunteers under the guidance of the Committee. Subcommittee III on Standard Spectral Data has the responsibility of preparing the ASTM-Wyandotte Spectral Data Index Cards. The chairman of this group is W. C. Kenyon, Hercules Powder Co., Wilmington, Del. Cooperating groups are the National Bureau of Standards, Battelle Memorial Institute, and other industrial, governmental, and academic laboratories. The spectral data activities are financed by funds from ASTM and by income from the sale of the index cards.

<u>Substances:</u> All in the literature or issued by other data gathering groups.

<u>Properties:</u> Separate card systems indexing near infrared, regular infrared, far infrared, visible, and ultraviolet absorption data are currently available or are being prepared.

Sources of Data: Catalogs of the American Petroleum Institute
Research Project 44, the Manufacturing Chemists Association Research
Project, the National Research Council Committee on Spectral Absorption
Data, Sadtler Research Laboratories, Documentation of Molecular Spectroscopy, and the Coblentz Society; current books and journals.

<u>Criticality</u>: The ASTM committee recommends the rerunning of samples when errors are detected in published spectra. A special form is available for customers to report errors found in the cards.

<u>Currency</u>: Attempts are made to keep up with literature and publications from established sources of spectral data.

Format: Each index consists of standard IBM cards punched according to a standard coding system so that a card corresponding to a given set of data (significant peaks in a spectrum or chemical structure) can be mechanically sorted on a standard IBM sorter. Each spectral card carries details of the absorption spectrum, complete description of chemical structure, a semi-empirical formula, melting or boiling point, and a reference to the source of the data. The Empirical Formula - Name Index Cards do not carry any absorption spectral data or organic structural information. These cards permit a search of the index by hand (or mechanical sorter) to determine whether the spectrum of a specific compound has been published. The information punched into the cards consists of the empirical formula, name and elements present, and reference code to permit location of the original data.

Publication and Distribution: Complete decks of cards and supplements, as they appear, may be purchased from the American Society for Testing Materials, 1916 Race Street, Philadelphia 3, Pa. As of March 1960 the deck of INFRARED SPECTRAL ABSORPTION INDEX CARDS contained 27,387 cards (purchase price, \$342.50) and the deck of ULTRAVIOLET SPECTRAL ABSORPTION INDEX CARDS, 10,933 cards (purchase price, \$137.50). The EMPIRICAL FORMULA — NAME INDEX CARDS TO INFRARED SPECTRA (purchase price, \$537.50) and the EMPIRICAL FORMULA — NAME INDEX CARDS TO ULTRAVIOLET SPECTRA (purchase price, \$232.50) cover the same spectra indexed in the spectral absorption decks.

VI. COMPREHENSIVE PROJECTS

VI-1. Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik, Technik

Organization: In 1883 Hans Landolt, with the collaboration of Richard Börnstein, issued the first edition (one volume) of PHYSIKALISCH-CHEMISCHE TABELLEN. Work on the sixth edition of LANDOLT-BÖRNSTEIN started soon after the last volume of the fifth edition was published in 1936. Publication began in 1950 under the editorship of the late Arnold Eucken. Editorial responsibility for recent volumes has been shared by J. Bartels, P. ten Bruggencate, H. Hausen, K. H. Hellwege, Kl. Schäfer, and E. Schmidt. Several parts are still in preparation.

Substances: Very wide coverage.

<u>Properties:</u> All important fundamental properties of physics, chemistry, astronomy, geophysics, and technology.

Sources of Data: World literature.

<u>Criticality</u>: Data for the sixth edition have been more critically examined than those in previous editions, but criticality in the best sense cannot be expected in such a massive undertaking.

<u>Currency</u>: Currency in the usual sense cannot be maintained in such a large compilation.

Format: The publication form is that of clothbound books. Data are presented in tables and graphs. Volumes are divided into parts, and tables of contents are given at the beginning of each part. In some places literature references are appended to the tables of data, and in other places they are found in general lists following the data. Compounds are arranged according to a system similar to that used by the American Petroleum Research Project 44, the Manufacturing Chemists Association Research Project, and the Circular 500 group of the National Bureau of Standards.

<u>Publication and Distribution:</u> Publisher of the sixth edition is Springer-Verlag, Berlin, Germany. The titles and approximate costs of volumes so far published and the titles of future volumes are as follows:

Landolt-Börnstein Volumes Published to Date

Vol. I: Atom-und Molekularphysik

- Part 1: Atome und Ionen; 1950; xii + 441 pp.; \$30.
- Part 2: Molekeln I: Kerngerüst; 1951; viii + 571 pp.; \$40.
- Part 3: Molekeln II: Elektronenhülle; 1951; xi + 724 pp.; \$52.
- Part 4: Kristalle; 1955; xi + 1007 pp.; \$76.
- Part 5: Atomkerne und Elementarteilchen; 1952; viii + 470 pp.; \$36.

Vol. II: Eigenschaften der Materie in ihren Aggregatzuständen

- Part 2a: Gleichgewichte, Dampf-Kondensat, Osmotische Phänomene; 1960; xi + 974 pp.; \$108.
- Part 3: Schmelzgleichgewichte und Grenzflächenerscheinungen; 1956; xi + 535 pp.; \$48.
- Part 6: Elektrische Eigenschaften I; 1959; xvi + 1018 pp.; \$108.
- Part 7: Elektrische Eigenshaften II; 1960; about 970 pp.; \$114.
- Vol. III: Astronomie und Geophysik; 1952; xviii + 795 pp.; \$60.

Vol. IV: Technik

- Part 1: Stoffwerte und mechanisches Verhalten von Nichtmetallen; 1955; xvi + 881 pp.; \$69.
- Part 3: Elektrotechnik. Lichttechnik. Röntgentechnik; 1957; xv + 1076 pp.; \$95.

Landolt-Börnstein Volumes in Preparation

Vol. II: Eigenschaften der Materie in ihren Aggregatzuständen

- Part 1: Mechanisch-thermische Zustandsgröszen
- Part 2b: Lösungsgleichgewichte I
- Part 2c: Lösungsgleichgewichte II
- Part 4: Kalorische Zustandsgröszen
- Part 5: Physikalische und chemische Kinetik: Akustik
- Part 8: Optische Konstanten
- Part 9: Magnetische Eigenschaften I
- Part 10: Magnetische Eigenschaften II

Vol. IV: Technik

Part 2: Metallische Werkstoffe

Part 4: Wärmetechnik

Also in the preparation or planning stages are three volumes on nuclear data.

<u>Comment:</u> It is unlikely that a total massive revision will be attempted again. Monographs on selected areas of science may be the mode of future publication.

VI-2. Tables de Constantes et Données Numériques Constantes Sélectionnées

Organization: Publication of TABLES ANNUELLES DE CONSTANTES ET DONNÉES NUMÉRIQUES began in 1909 under the aegis of the International Union of Pure and Applied Chemistry and the editorship of C. Marie. The tables were to bring together all the numerical data published in chemistry, physics, biology, and technology. Ten volumes appeared between 1910 and 1930, and these were indexed in two separate volumes. Volumes XI (1931-34) and XII (1935-36) consisted of 8 and 12 sections, respectively, on special topics. In 1947 publication resumed under the title TABLES DE CONSTANTES ET DONNÉES NUMERIQUES. CONSTANTES SÉLECTIONNÉES. To date expert collaborators have compiled eleven numbered monographs in this new series. Present editor-in-chief is Madam S. Allard, 18 rue Pierre Curie, Paris Ve, France. Because "Tables de Constantes" is an affiliated commission of IUPAC, there has been much international collaboration. Until 1955 the chief source of financial support was a subvention from IUPAC. Since then the organization has become largely self-supporting through the sale of its volumes. "Tables de Constantes" now has an arrangement with Pergamon Press whereby Pergamon advances money for preparing a table and later markets the completed volume.

<u>Substances</u>: The substances covered in a given monograph are related to the property or properties of interest.

<u>Properties:</u> The list of publications below shows the variety of properties covered since 1947. In recent years efforts have been directed toward rapidly moving fields of science. For example, tables on radiolytic yields and the properties of semi-conductors are currently in preparation.

Sources of Data: World literature.

<u>Criticality</u>: There is some selection of values, but the criticality varies from one monograph to another. The goal is to produce "useful" values.

Use of Nomenclature, Symbols, Units, Physical Constants: Affiliation with IUPAC facilitates consultation and collaboration with experts.

<u>Currency</u>: Early monographs in the current series have not been brought up to date. However, future plans call for issuing supplements to some of the more recent publications. For example, in 1961 there will be a supplement to the 1956 publication on the optical rotatory power of steroids.

Format: The data are presented mostly in tables. Arrangement of material varies since different substances and properties are treated in each monograph. The publications have been paper-covered until recently; the last four numbers have hard covers. General indexes are sometimes given. A bibliographic column in the tables guides the user to the pertinent literature reference in the general bibliography at the end of the monograph.

Publication and Distribution: In the present series (since 1947) there have been several publishers. Numbers 1 through 5 were published by Hermann & C^{ie}, 6 and 7 by Masson & C^{ie}, and 8 through 11 by Pergamon Press. A list of titles with authors, dates, and prices follows. All the volumes can now be purchased from Pergamon Press, 122 East 55th Street, New York 22, N. Y.

List of Publications since 1947 Tables de Constantes et Données Numériques

- Longueurs d'onde d'émissions X et des discontinuités d'absorption X, par Y. Cauchois et H. Hulubei; 1947; 199 pp.; \$4.50.
- Physique nucléaire, établi par R. Grégoire, sous la direction de F. Joliot et I. Curie; 1948; 131 pp.; \$6.00.
- Pouvoir rotatoire magnétique (Effet Faraday), par R. De Mallemann; Effet magnéto-optique de Kerr, par F. Suhner; 1951; 137 pp.; \$4.50.
- Données spectroscopiques concernant les molécules diatomiques, établi par R. F. Barrow, A. D. Caunt, A. R. Downie, R. Herman, E. Huldt, A. McKellar, E. Miescher, B. Rosen et K. Wieland; rédaction générale, B. Rosen; 1951; 361 pp.; \$15.00.

- Atlas des longueurs d'onde caractéristiques des bandes d'émission et d'absorption des molécules diatomiques, par R. F. Barrow, A. D. Caunt, A. R. Downie, R. Herman, E. Huldt, A. McKellar, E. Miescher, B. Rosen et K. Wieland; rédaction générale, B. Rosen; 1952; 389 pp.; \$17.50.
- Pouvoir rotatoire naturel. I. Steroides, par J.-P. Mathieu et A. Petit; 1956; 507 pp.; \$36.00.
- 7. Diamagnétisme et Paramagnétisme, par G. Foëx; Relaxation paramagnétique, par L.-J. Smits et C.-J. Gorter; 1957; 317 pp.; \$29.00.
- 8. Potentiels d'oxydo-réduction, par G. Charlot, D. Bézier et J. Courtot; 1958; 41 pp.; \$5.00.
- Pouvoir rotatoire naturel. -- II. Triterpènes, par J.-P. Mathieu et G. Ourisson; 1958; 302 pp.; \$21.00.
- Pouvoir rotatoire naturel. -- III. Amino-acides, par J.-P. Mathieu, P. Desnuelle, et J. Roche; 1959; 61 pp.; \$6.50.
- 11. Pouvoir rotatoire naturel. -- IV. Alcaloïdes, par J.-P. Mathieu et M.-M. Janot; 1959; 211 pp., \$24.00.

INDEX OF COMPOUND TYPES IN SECTIONS I, II, IV, AND V

Projects following (a) cover the whole substance class or all the substances in the class to which the given property is applicable; projects following (b) cover a limited part of the substance class.

Inorganic compounds (including elements)

Chemical kinetics properties
Crystallographic properties
Phase diagrams
Physical properties
Spectral properties
atomic spectra
infrared spectra
mass spectra
NMR spectra
Raman spectra
ultraviolet spectra
visible spectra
Thermodynamic properties

Organic compounds

Chemical kinetics properties
Crystallographic properties
Physical properties
Spectral properties
infrared spectra

Thermophysical properties

mass spectra
NMR spectra
Raman spectra
ultraviolet spectra
visible spectra
Thermodynamic properties
Thermophysical properties

Project number

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- (a) I-5
- (a) I-4; II-5; (b) II-1,4
- (a) V-A-1
- (a) V-B-4, 5, 7; V-G-1; (b) V-B-3, 8
- (a) V-D-2
- (a) V-F-2
- (a) V-E-2
- (a) V-C-2, 3; V-G-1
- (a) V-C-3; V-G-1
- (a) I-4,7; (b) I-3,6,8
- (a) IV-3; (b) IV-1,2
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- (b) V-B-1, 2, 7
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