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Continuing Numerical Data Projects: A Survey and Analysis (1966)

Pages
227

Size
5 x 9

ISBN
030934056X

Office of Critical Tables; National Research Council

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CONTINUING NUMERICAL DATA PROJECTS

A SURVEY AND ANALYSIS

N.R.C. OFFICE OF CRITICAL TABLES
NATIONAL ACADEMY OF SCIENCES
NATIONAL RESEARCH COUNCIL

SECOND EDITION

PUBLICATION 1463
National Academy of Sciences National Research Council
WASHINGTON, D.C.
1966

Z 7405
.T3 N35
1966
C.1

Available from

Printing and Publishing Office
National Academy of Sciences
2101 Constitution Avenue
Washington, D.C. 20418

Price: $5.00

Library of Congress Catalog Card Number: 66-62211

Foreword

It is becoming more and more apparent that publication of critical tables of standard reference data is one of the most important aspects of retrieval from the scientific literature of the results of scientific research. Such tables have long been recognized as essential for the efficient progress of science and technology. Thus it is particularly gratifying to have a 1966 revision of "Continuing Numerical Data Projects—A Survey and Analysis," first published in 1961 under the auspices of the Office of Critical Tables of the National Academy of Sciences - National Research Council.

The new volume describes the operations and publications of more than 50 active projects engaged in the compilation of data. This is a significant increase over the content of the 1961 volume and reflects the growing involvement of the scientific community in the problem of data for science and technology. Most of the projects are in the United States but some important ones are in other countries. A few of them result from international collaboration.

Although the total coverage of the projects described in this new volume is not as great as that of the International Critical Tables (ICT), the coverage of most of the individual areas of the projects described is in greater depth and more detail than the corresponding parts of the ICT. As current national and international plans for establishment of new data-compiling projects get under

way, the number of continuing numerical data projects will increase. In the foreseeable future, a sufficient number of programs should be created to provide compilations for all significant areas of the physical sciences. When that state of affairs comes about, the ICT will have been revised in the manner envisioned by the Office of Critical Tables when it was established in 1957. All useful quantitative scientific data will be available in recognized collections of numerical data for science and technology, and a mechanism for the continual updating of each collection will exist.

The present volume will serve as the starting point for a more comprehensive worldwide survey of resources for evaluating and compiling numerical data. This worldwide survey will be started immediately by the Committee on Data for Science and Technology of the International Council of Scientific Unions through its Central Office which is presently located in Washington, D.C.

Greatest credit for this volume goes to Dr. Miriam G. Buck, the Editor, without whose painstaking efforts the work could not have been completed. Thanks are also extended to Dr. Guy Waddington, Director of the NAS - NRC Office of Critical Tables, who supervised the work, to the project directors in the United States and abroad who reviewed the individual sections, and to Mrs. Alice MacIntyre and Mrs. Gloretta Bishop for their careful typing and preparation of the manuscript. Special thanks are due to the National Science Foundation and the Office of Standard Reference Data of the National Bureau of Standards for their support of the work.

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

The Office of Critical Tables

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

Chairman:

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

Chemistry and Chemical Technology:

J. L. Margrave, Professor of Chemistry, The Rice University

Earth Sciences:

James R. Balsley, Professor of Geology, Wesleyan University

Engineering:

Karl L. Fetters, Vice-President, Research and Development, The Youngstown Sheet and Tube Co.

Antoine M. Gaudin, Richards Professor of Mineral Engineering Emeritus, Massachusetts Institute of Technology

George E. Holbrook, Vice-President, E. I. du Pont de Nemours & Co., Inc.

Physical Sciences:

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

Ex officio:

Allen V. Astin, Director, National Bureau of Standards

The Executive Committee of the Office also serves as the U.S. National Committee for the newly established Committee on Data for Science and Technology of the International Council of Scientific Unions and as the Review Committee for the National Standard Reference Data Program of the National Bureau of Standards.

The Office staff develops and carries out the general program outlined by the Executive Committee. As of October 1966 the staff included the following professional members: Guy Waddington, Director; Hendrik van Olphen, Assistant Director; and Miriam G. Buck, Research Associate.

The Advisory Board of the Office, which is a source of expert knowledge in the many areas of compilation activities, consists of about 65 members. It is composed 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 Aeronautics and Astronautics
American Institute of Chemical Engineers
American Institute of Mining, Metallurgical, and Petroleum Engineers
American Institute of Physics
American Meteorological Society
American Oil Chemists' Society
American Physical Society, The
American Society for Engineering Education, The
American Society for Metals
American Society for Testing and Materials
American Society of Biological Chemists
American Society of Civil Engineers
American Society of Heating, Refrigerating, and Air Conditioning Engineers, Inc.
American Society of Mechanical Engineers, The
Electrochemical Society, Inc.
Geochemical Society, The
Geological Society of America, The
Illuminating Engineering Society
Institute of Electrical and Electronic Engineers, The
Mineralogical Society of America
Optical Society of America
Seismological Society of America
Society of Automotive Engineers, Inc.
Society of Economic Geologists, Inc.
Society of Naval Architects & Marine Engineers, Inc.
Special Libraries Association

B. INDUSTRIAL ASSOCIATIONS

Aerospace Industries Association
American Iron and Steel Institute
American Petroleum Institute
Industrial Research Institute, Inc.
Manufacturing Chemists Association, Inc.
Textile Research Institute

C. UNITED STATES GOVERNMENT

Agricultural Research Service, Department of Agriculture
Air Force Materials Laboratory
Air Force Office of Scientific Research
Army Research Office (Durham)
Bureau of Mines, Department of the Interior
Bureau of Reclamation, Department of the Interior
Coast and Geodetic Survey, Department of Commerce
Defense Documentation Center
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

Contents

Introduction

For more than 40 years the National Academy of Sciences has regarded critical tables of reference data as of key importance in the literature of science. This concern was reflected very early by its leadership in producing the International Tables of Numerical Data (see Section 5.3.). Formation of the Office of Critical Tables (OCT) in 1957 was another expression of the Academy's awareness of the need for continuing action to supply the scientific and technological communities with reliable tables of numerical data.

One of the important functions of OCT has been to survey the status of the efforts made by compilers in all countries to evaluate, compile, and publish systematically data for all areas of the physical sciences on a continuing basis. The results of an initial survey were published in 1961, and the present volume is a revision of the earlier work. The Survey has several purposes. It is an aid to planners of compilation programs in avoiding overlap of effort, in identifying gaps where work should be initiated, and in appraising standards of performance. It is helpful to individuals, librarians, and technical information personnel in identifying sources of authoritative numerical data. Only broad categories of information are presented, such as thermodynamic data, spectroscopic data, and crystallographic data; and for substances, categories such as inorganic or organic

1
Thermodynamic, Thermophysical, and Physicochemical Projects

1.1. THERMODYNAMIC PROJECTS

1.1.1. SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES: NBS CIRCULAR 500

Organization

This project, well known for its publication of the classic NBS Circular 500, is carried out in the Physical Chemistry Division of the Institute for Basic Standards of the National Bureau of Standards (NBS) and is now an important unit of the National Standard Reference Data Program. It has functioned since 1940 and since 1950 has been under the direction of Donald D. Wagman. The activity has been supported in part by the Office of Naval Research and the U. S. Atomic Energy Commission and more recently by the Office of Standard Reference Data.

1.1.1.

Substances

The program includes all elements, inorganic compounds, C_1 and C_2 organic compounds, aqueous solutions of important acids, bases and salts, and some gaseous and aqueous ions.

Properties

The tables are grouped in three series. Series I gives values at 25° C for heat (enthalpy), Gibbs energy and logarithm of equilibrium constant of formation, entropy, and heat capacity, and for a few substances, values for heat of formation at 0° K. For solutions of important salts, thermodynamic properties are given at concentrations from near saturation to infinite dilution. Series II gives change-of-phase values, i.e., temperature, heat, entropy, heat capacity, and some pressure values. Series III gives values at temperatures from 0° to 5,000° K for enthalpy, Gibbs energy, logarithm of equilibrium constant of formation, Gibbs energy function, heat content function, entropy, heat content (enthalpy), and heat capacity. Only Series I and II are included in Circular 500. In the revised tables, published as Technical Notes, log Kf is omitted and the enthalpy at 298.15° K is given.

Sources of Data

Primary research papers published in the literature provide the main source of information. Unpublished research reports are used to a limited extent.

Critical Appraisal

The tables are internally consistent in that all known physical and thermodynamic relations existing between different properties of a substance, or the same property for different substances, are satisfied by the tabulated values. Recorded values are not necessarily those appearing in any one reference but may have been calculated after a careful evaluation of all available experimental data, using consistent values for all subsidiary quantities. The 25° C values presented by this project constitute a base on which all thermodynamicists depend. No complete index is given, but the tables are arranged

according to the Standard Order System, which is explained in the introduction. An alphabetical list of elements with their table numbers enables tables for a given element to be easily located. Specific references for each entry in the tables are tabulated on separate sheets and are followed by a complete general list of references. Technical Note 270-1 contains a descriptive introduction but no references. Technical Note 270-2 has only tables. References and discussion of the sources will be included in the complete revision of the tables of Series I.

Use of Nomenclature, Symbols, Units, and Physical Constants

Usages prescribed by international committees and bodies such as the International Union of Pure and Applied Chemistry (IUPAC) are followed. In the revision of Circular 500, use will be made of the 1963 fundamental constants and of the ^{12}C atomic weight scale. In the introduction, values of energy units and fundamental constants are given, symbols and abbreviations are defined, and conventions regarding standard states are explained.

Currency

From March 31, 1947, to March 31, 1950, tables for Series I and II were issued quarterly. Coverage of the literature to 1950 was good, as evidenced by the esteem in which Circular 500 is held and the need for a reprinting in 1961. The staff continues to survey the current literature, seeking and evaluating data suitable for inclusion in their tables or for modification of older data. Wide areas have been somewhat neglected in favor of selected special elements and compounds. No loose-leaf sheets for Series I and II have been issued since 1950, but some Series III sheets were issued as late as March 1956. Circular 500 is being revised and issued as a series of interim publications in the form of NBS Technical Notes in order to make the tables available as soon as possible. Revised Tables 1 - 32 have been issued.

Format

The loose-leaf sheets, the bound volume, and the recently published Technical Notes are 8" x 10 1/2". A two-part paperback photo-

reprint of Circular 500, 5 7/8" x 9", was made in 1961. Series I sheets precede those of Series II.

Publication and Distribution

Selected Values of Chemical Thermodynamic Properties, NBS Circular 500, 1952, iv + 1,268 pp. (out of print). Paperback reprint issued in two parts: I. Tables; and II. References; 1961 (out of print).

Selected Values of Chemical Thermodynamic Properties

Part 1: Tables for the First Twenty-three Elements in the Standard Order of Arrangement, NBS Technical Note 270-1, D. D. Wagman et al., Oct. 1965, iv + 124 pp., 65 cents.

Part 2: Tables for the Elements Twenty-four Through Thirty-two in the Standard Order of Arrangement, NBS Technical Note 270-2, D. D. Wagman et al., May 1966, iv + 62 pp., 40 cents.

Note: Technical Note 270-1 contains only the C_1 compounds of Table 23. The C_2 compounds (and possibly additional C_1 compounds) will be issued as Technical Note 270-1a. The complete revision of the tables of Series I will be published as a contribution in the National Standard Reference Data Series.

Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

1.1.2. SELECTED VALUES OF PROPERTIES OF HYDROCARBONS AND RELATED COMPOUNDS (Category A, Physical and Thermodynamic Properties): American Petroleum Institute Research Project 44

Organization

This project, established in 1942 at the National Bureau of Standards in Washington D.C., moved in 1950 to the Carnegie Institute of Technology in Pittsburgh, Pa., and again in April 1961 to the Chemical Thermodynamic Properties Center, now the Thermodynamics Research Center, Texas A&M University, College Station, Texas. The project has been sponsored and financed by the American Petroleum Institute (API) continuously since its inception. Frederick D. Rossini directed the project until 1960 when Bruno J. Zwolinski succeeded him. The staff of approximately eight includes both full- and part-

time professional workers, plus supporting editorial and office help. An API-appointed Advisory Committee provides scientific guidance and liaison with sponsors. API Research Project 44 compiles and publishes information on physicochemical and thermodynamic property values, and infrared, ultraviolet, mass, Raman, and nuclear magnetic resonance spectroscopic data.

Substances

Aliphatic and aromatic hydrocarbons; oxygen-containing compounds such as alcohols, aldehydes, ketones, ethers, and alkanoic acids; sulfur derivatives such as thial-alkanes, thiols, and alkyl thiopenes; and a few important simple substances like O_2, N_2, CO_2, and H_2O that enter into many computations.

Properties

Values for each substance listed are given for the following physicochemical and thermodynamic properties: boiling point; dt/dp; freezing point; refractive index; molal and specific refraction; refractivity intercept; density; specific gravity; vapor pressure; specific dispersion; surface tension; absolute and kinematic viscosity; isothermal compressibility coefficient; compressibility factor and activity coefficient of gases; critical temperature, pressure, density, volume, and compressibility factor; Gibbs energy (free energy); Gibbs energy function; heat, entropy, and temperature of phase changes; heat of combustion; heat, Gibbs energy and logarithm of equilibrium constant of formation; standard entropy; heat content; heat content function; heat capacity; enthalpy, entropy, and Gibbs energy deviations from ideal or standard state values for gases. Property values are presented at standard reference points, or at selected even intervals of the variables (temperature, pressure, etc.) over ranges dictated by probable use of the data and reliability of the extrapolation methods. (The spectral programs of API-RP 44 are described in Sections 4.2.1., 4.3.1., 4.4.1., 4.5.1., and 4.6.1.)

Sources of Data

Primarily papers from the open literature; selected unpublished data from contributing industrial, academic, and governmental laboratories.

1.1.2.

Reliable correlations and quasi-theoretical computational methods are used to derive property values in inaccessible temperature ranges or when experimental data are not available.

Critical Appraisal

Careful evaluation of all available data and use of tested correlation methods ensure that tabulated values are as reliable as possible, frequently better than source data. The introduction to the publication includes a discussion of criteria applied in making selections and equations employed to obtain computed values. Computational techniques featured are extrapolation and interpolation by tested methods, calculation of derived thermodynamic functions from spectroscopic and molecular structure data, and extension of experimental values by way of molecular structure similarities. A table applicable to most of the recorded properties gives the magnitudes of estimated uncertainties in the values. Internal consistency within related bodies of information is maintained.

Use of Nomenclature, Symbols, Units, and Physical Constants

Recommendations of national and international committees on nomenclature and symbols are followed. The introductory material is admirably complete in giving definitions of properties, values of fundamental and derived constants, and unit conversion factors. All data taken from the literature are carefully conformed to consistent units. Newly recommended values for constants and atomic weights are introduced into revisions only when internal consistency can be maintained. For the benefit of engineers, separate tables are given in English units when appropriate.

Currency

Revisions and additions are issued semiannually. The loose-leaf format permits regular updating so that the file of information always includes the most recent values. In many instances, previously unpublished data are made available to the scientific public in less time than through regular (journal) channels.

Format

The primary form of publication is the 8" x 10 1/2" loose-leaf sheet for which special post binders are available. Physicochemical and thermodynamic property values are tabulated on one side of the sheet. Each sheet gives the identifying table number and title, the names and molecular formulas of the compounds for which values are given, the names and units of property values, and the dates of original issue and revisions. Pages are not numbered. Instead, the properties are grouped in tables designated a, b, c, etc.; in each group pages are arranged in an order based on the Standard Order System and in turn on unsaturation (hydrocarbons) and group classification (nonhydrocarbons). Complete directions for filing that permit maintenance of an ever-current, correctly ordered set are issued in a separate publication (see following section). No references are given on the data sheets, but two types of reference sheets are provided, specific and general, that permit identification of all sources of background data. A new cumulative "General List of References," with 7,351 entries, was issued April 30, 1963. Bound volumes consolidating the then current values of physicochemical and thermodynamic properties of the tables were published in 1947 and in 1953.

Publication and Distribution

Selected Values of Properties of Hydrocarbons, NBS Circular 461, 1947, xiii + 483 pp. (out of print).

Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, Carnegie Press, 1953, ix + 1,050 pp. (out of print)

Selected Values of Properties of Hydrocarbons and Related Compounds, current loose-leaf sheets. As of June 30, 1966, there were 2,391 valid sheets of which approximately 1,867 are tables containing data on more than 3,100 compounds. Complete set, 6 volumes.

A supplementary publication, "Suggested Procedures Regarding the Arrangement, Filing, and Maintenance of the Loose-leaf Sheets in the Tables and Spectral Catalogs of the American Petroleum Institute Research Project 44," is available to prospective and current recipients of the sheets.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas. Member

companies of API may receive them on a subscription basis and may obtain additional sets at a reduced rate. On request, university departments, certain cooperative United States government laboratories, nonprofit institutions, and independent libraries may receive single sets provided the organization agrees to payment of (1) an initial set fee of about 10 percent of the normal price for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested may purchase the sheets in complete sets only, at 30 cents per sheet. Initial sets are now completely collated in attractive, durable API binders.

1.1.3. SELECTED VALUES OF PROPERTIES OF CHEMICAL COMPOUNDS (Category A, Physical and Thermodynamic Properties): Manufacturing Chemists Association Research Project

Organization

The Manufacturing Chemists Association (MCA) Research Project was established in 1955 at the Carnegie Institute of Technology in Pittsburgh, Pa. In 1961 the project was moved to the Chemical Thermodynamic Properties Center, now the Thermodynamics Research Center (TRC), Texas A&M University, College Station, Texas. Frederick D. Rossini directed the project until 1960 when Bruno J. Zwolinski succeeded him. Through 1963 MCA was the sponsor. In 1964 the National Bureau of Standards, through the Office of Standard Reference Data, joined in giving financial support. The staff of approximately a dozen, includes both full-time and part-time professional workers, plus supporting editorial and office staff. An advisory committee provides guidance and liaison with industry. The MCA Research Project compiles and publishes information on physicochemical and thermodynamic property values, and infrared, ultraviolet, mass, Raman, and nuclear magnetic resonance spectroscopic data.

Substances

Inorganic and organic compounds of importance to the chemical industry and science in general. Included to date are nonmetallic elements and their inorganic compounds, oxygen-containing organic

compounds (alkanols, phenols and xylenols, and alkanoic acids) and nitrogen- and halogen-substituted acyclic compounds. Since the project is complementary to API Research Project 44, hydrocarbons and certain related nitrogen and sulfur compounds covered by that project are excluded.

Properties

The plan is to cover the same properties as those covered by API Research Project 44 (see Section 1.1.2.). To date, numerical values are presented for the following properties: (1) refractive index, density, boiling point, dt/dp, freezing point; (2) density for the normal liquid range of temperatures at 1 atmosphere; (3) critical temperature, pressure, density, volume, and compressibility factor; (4) vapor pressures and boiling points at 10 - 1,500 mm Hg; (5) enthalpy, temperature, entropy, and heat capacity phase changes, cryoscopic constant; and (6) enthalpy and Gibbs energy functions, entropy, enthalpy and heat capacity for the ideal gas at 0 - 1,500° K. (The spectroscopic programs of MCA are discussed in Sections 4.2.2, 4.3.2, 4.4.2, 4.5.2, and 4.6.2.)

Sources of Data

Primarily papers from the open literature, also selected unpublished data furnished by contributing laboratories. Reliable correlating and quasi-theoretical computational methods are used to derive property values when experimental data are not available and to extend the temperature range.

Critical Appraisal

Careful evaluation of available data and the use of tested correlation methods ensure that tabulated values are as reliable as possible, frequently better than source data. Internal consistency within related bodies of information is maintained. The selection of a value for a given compound may be done in the context of data for a group of structurally related compounds. The reliability of the individual values is enhanced through correlation with molecular structure. Such correlations may provide reliable values for properties that have

not been measured and for compounds that may not yet have been isolated or prepared in the laboratory.

Use of Nomenclature, Symbols, Units, and Physical Constants

Recommendations of national and international committees on nomenclature and symbols are followed. The introduction to the compilation contains a summary statement of the units in which property values are given.

Currency

Revisions and additions are issued periodically, with the goal of semiannual issue of supplements. The loose-leaf format permits regular updating so that the file of information always includes the most recent values. 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.

Format

All data are presented in tables on 8" x 10 1/2" loose-leaf sheets for which special post binders are available. The sheets are arranged according to titles and letters representing certain properties. Within a given section, sheets are arranged according to the Standard Order System, based on the periodic table. No references are given on the data sheets, but two types of reference sheets are provided, specific and general, that permit identification of all sources of background data. Unpublished values created by the project by appropriate calculation and correlation are referenced as MCA Research Project (calculated values).

Publication and Distribution

Selected Values of Properties of Chemical Compounds, current loose-leaf sheets. As of June 30, there were 754 valid sheets, of which 335 were tables containing data on over 1,900 compounds. Complete set, 2 volumes.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas. The loose-leaf data sheets are available free in complete sets to all educational institutions of higher learning and certain United States government research laboratories, provided the organization agrees to payment of (1) an initial set fee of about 10 - 15 percent of the normal cost for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested, such as private institutions, independent libraries, and foreign governments, should contact the Texas A&M Data Distribution Office regarding discount susbscription rates. Initial sets are now completely collated in attractive, durable binders. Member companies of MCA and all other industrial organizations may receive the MCA data sheets on a subscription basis. Additional complete sets of loose-leaf data sheets may be purchased at 30 cents per sheet.

Effective July 1, 1966, the MCA loose-leaf data sheets prepared by the Thermodynamics Research Center, Department of Chemistry, Texas A&M University, will be known as TRC data sheets.

1.1.4. JANAF THERMOCHEMICAL TABLES

Organization

The JANAF Thermochemical Tables project was established at the Dow Thermal Research Laboratory, Midland, Mich., under contract with the Advanced Research Project Agency (ARPA) in late 1959. D. R. Stull is the project director. The purpose of the project is to compile and publish consistent tables of thermochemical data required for propellant performance calculations. Technical advice and guidance have been provided by a group of expert consultants. A related experimental program, also supported by ARPA in a number of laboratories, has provided missing data and the redetermination of questionable values. Since 1964 the project has been supported by the U.S. Air Force, Edwards Air Force Base.

Substances

The aim of the project is to cover thermodynamic properties of the first 17 elements in the Periodic Table and their relevant compounds,

principally those with the halogens, oxygen, and hydrogen, and with mixed salts containing sodium and potassium. Some compounds containing mercury, iodine, phosphorus, titanium, tungsten, and zirconium are also included, as well as properties of the elements contained in the compounds.

Properties

The properties given in table form are heat capacity, entropy, Gibbs (free) energy function, heat content (enthalpy), heat of formation, and Gibbs energy of formation for the ideal gas, liquid or solid state as appropriate. The logarithm of equilibrium constant of formation of each compound from the elements in their standard reference states is also given. These properties are given at 100-degree intervals from 0°K to 1,000 - 6,000°K. Other pertinent properties are presented, such as molecular weight, point group, ground state configuration or quantum weight, vibrational frequencies and degeneracies, bond distances and angles, and product of the moments of inertia.

Sources of Data

Open literature, private communications, and to some extent empirical and quasi-theoretical computations, and estimates obtained by various means to fill in gaps.

Critical Appraisal

Property values for each element and compound are evaluated from all available data that are relevant. An effort is made to maintain internal consistency among all the data presented. Some of the values, particularly early ones, were estimates based on inadequate supporting data. Pertinent references, a brief analysis of available data, and the basis for the selections made are also given. The introduction includes explanations of and equations for methods used to compute values needed to fill gaps in the experimental data. An effort is made to eliminate questionable values by a system of review before incorporation into the collection.

Currency

Formerly, revisions and additions to the JANAF Tables were issued quarterly to a limited number of qualified users. In August 1965, the existing tables, with data up to July 1965, were published by the U.S. Department of Commerce Clearinghouse for Scientific and Technical Information and are available to the public. Periodically the tables will be updated and revised, and supplements will be issued. This compilation has succeeded in utilizing recently published and unpublished data.

Use of Nomenclature, Symbols, Units, and Physical Constants

All symbols used are defined; values and units are given for basic, derived, and defined constants. The uncertainty in values for basic and derived constants is also given. (The constants used are largely those of Cohen, Crowe, and Dumond, "The Fundamental Constants of Physics," 1957.)

Format

The Clearinghouse issue consists of 8 1/2" x 11" loose-leaf sheets, with a lightweight paper cover. The numerical data and other information for a given substance or state of a substance are set in parallel columns on a page. The formulas of compounds are written according to the modified Hill (Chemical Abstracts) system. This is an alphabetical arrangement of the chemical symbols in the formulas except for carbon compounds when C is placed first, followed by H if hydrogen is also present. Pages are ordered alphabetically according to the Hill formula of the compounds. No page numbers are required, and revisions and additions can be accommodated.

Publication and Distribution

JANAF Thermochemical Tables, PB 168 370, 1965, 945 pp., $10.00. Supplements 18, 19, 20, and 21, PB 168 370-1, announced as available in Aug. 1966, $4.00.

Available from Clearinghouse for Scientific and Technical Information, U.S. Department of Commerce, Springfield, Va. 22151.

The tables are now available on magnetic tape to persons or installations approved by the director and the sponsoring agency. Persons wishing to know the price of these tapes, and the qualifications required for obtaining them may write to Dr. Harold Prophet, Thermal Research Laboratory, 1707 Building, The Dow Chemical Company, Midland, Mich. 48640.

1.1.5. CONTRIBUTIONS TO THE DATA ON THEORETICAL METALLURGY: Bureau of Mines

Organization

The Bureau of Mines has supported thermodynamic work at the Berkeley Thermodynamics Laboratory on the University of California campus, Berkeley, Calif., since the early 1920's. Compilation of thermodynamic data was started in the early 1930's, and soon after World War II the laboratory became entirely devoted to thermodynamic work. Financial support is provided by appropriations from the Department of the Interior. The program at Berkeley was directed by K. K. Kelley from 1930 until his retirement in 1964. The Bureau of Mines plans to continue the work. An integrated program of precision thermodynamic measurements is associated with the compilation activity, thus providing the staff with the experience necessary for critical evaluation of data.

Substances

All the elements and their inorganic compounds that are of interest in metallurgical and ceramic operations, including oxides, halides, carbides, carbonates, sulfides, sulfates, nitrates, nitrides, and some intermetallic and interoxidic compounds.

Properties

Gibbs energy (free energy), entropy, heat content (enthalpy), high and low temperature heat capacity, heat and free energy of formation and phase change, and vapor pressure. The values compiled are those needed for the thermodynamic evaluation of metallurgical processes.

Sources of Data

Primarily the open literature; to a limited extent unpublished measurements made at the Berkeley Laboratory.

Critical Appraisal

Specific thermodynamic property values are selected after a critical evaluation of all available experimental and calculated values. Complete references are cited, and those given the greatest weight are italicized. Estimated uncertainties are given when possible. A critical discussion of source data and of equations used for calculations is often given. The continuing 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, and Physical Constants

Recommendations of authoritative national and international committees are followed.

Currency

Periodically, bulletins are revised on important topics such as low and high temperature heat capacities and entropies for oxides. However, the pattern of publication (i.e., bulletins at intervals of several years) does not provide a continued updating of all topics included in the program.

Format

Earlier issues of this paperback series were 5 3/4" x 9 1/8"; more recent ones are 7 3/4" x 10 1/4". Data are presented in tables or in textual form, or both. Elements and their compounds are arranged alphabetically, and the bibliographies, are also alphabetical, arranged by author.

1.1.5.

Publication and Distribution

Contributions to the Data on Theoretical Metallurgy, I - XV, from the Berkeley Laboratory.

Published as Bureau of Mines bulletins between 1932 and 1962. Six of the bulletins are revisions, and Bulletin 601 is a reprinting of four previous bulletins out of print for some years but still in demand as essential in present-day research. A complete current set of data includes Bulletins 407 and 542 (both out of print), 584, 592, and 601.*

In addition to the bulletins, numerous pamphlets on individual thermodynamic properties of a particular substance or similar compounds of several elements have been issued as Reports of Investigations. Though the editions are limited, single copies of most of them are available free from the Publications Distribution Section, Pittsburgh, Pa.† Monthly lists, "New Publications, Bureau of Mines," annual lists, and cumulative lists of publications are also issued. Several reports of investigations have been compilations of thermodynamic properties of a given element and its compounds.

Publications

Contributions to the Data on Theoretical Metallurgy

I. The Entropies of Inorganic Substances, K. K. Kelley, Bulletin 350, Bureau of Mines, 1932, 63 pp. Superseded by VI, IX, XI, and XIV.

II. High-Temperature Specific-Heat Equations for Inorganic Substances, K. K. Kelley, Bulletin 371, Bureau of Mines, 1934, 78 pp. Superseded by X and XIII.

III. The Free Energies of Vaporization and Vapor Pressures of Inorganic Substances, K. K. Kelley, Bulletin 383, Bureau of Mines, 1935, 132 pp. Reprinted in XV.

IV. Metal Carbonates, Correlation and Applications of Thermodynamic Data, K. K. Kelley and C. T. Anderson, Bulletin 384, Bureau of Mines, 1935, 73 pp. Reprinted in XV.

V. Heats of Fusion of Inorganic Substances, K. K. Kelley, Bulletin 393, Bureau of Mines, 1936, 166 pp. Reprinted in XV.

VI. A Revision of the Entropies of Inorganic Substances—1935, K. K. Kelley, Bulletin 394, Bureau of Mines, 1936, 55 pp. Superseded by IX, XI, and XIV.

VII. The Thermodynamic Properties of Sulphur and Its Inorganic Compounds, K. K. Kelley, Bulletin 406, Bureau of Mines, 1937, 154 pp. Reprinted in XV.

VIII. The Thermodynamic Properties of Metal Carbides and Nitrides, K. K. Kelley, Bulletin 407, Bureau of Mines, 1938, 66 pp. (out of print).

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. Superseded by XI and XIV.

X. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for Inorganic Compounds, K. K. Kelley, Bulletin 476, Bureau of Mines, 1949, 241 pp. Superseded by XIII.

XI. Entropies of Inorganic Substances, revision (1948) of Data and Methods of Calculation, K. K. Kelley, Bulletin 477, Bureau of Mines, 1950, 147 pp. Superseded by XIV.

XII. Heats and Free Energies of Formation of Inorganic Oxides, James P. Coughlin, Bulletin 542, Bureau of Mines, 1954, 80 pp. (out of print).

XIII. High-Temperature Heat-Content, Heat Capacity, and Entropy Data for the Elements and Inorganic Compounds, K. K. Kelley, Bulletin 584, Bureau of Mines, 1960, 232 pp., $1.25.*

XIV. Entropies of Elements and Inorganic Compounds, K. K. Kelley and E. G. King, Bulletin 592, Bureau of Mines, 1961, 149 pp., 75 cents.*

XV. A Reprint of Bulletins 383, 384, 393, and 406 (III, IV, V, and VII), Bulletin 601, Bureau of Mines, 1962, 525 pp. †

Reports of Investigations

R. I. 5490—Metallurgical Thermochemistry of Titanium, K. K. Kelley and A. D. Mah, 1959, 48 pp., 30 cents.*

R. I. 5600—Thermodynamic Properties of Manganese and Its Compounds, A. D. Mah, 1960, 35 pp., 30 cents.*

* Bulletins 584 and 592 and Reports of Investigations 5490 and 5600 may be obtained from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

† Single copies of Bulletin 601 and pamphlets may be obtained free from the Publications Distribution Section, Bureau of Mines, 4800 Forbes Ave., Pittsburgh, Pa. 15123.

1.1.6. CONTINUING CHEMICAL THERMODYNAMIC COMPILATIONS OF THE SOVIET UNION

In the Soviet Union two related continuing programs for the systematic evaluation and publication of thermodynamic properties of elements and their compounds are being carried out under the aegis of the USSR Academy of Sciences. V. P. Glushko is chief editor of both publications. One program, "Thermodynamic Properties of Chemical Substances," covers the thermodynamic properties of elements

and simple inorganic compounds over a wide range of temperatures. The other, "Thermodynamic Constants of Substances," is concerned with the thermodynamic properties at 298.15°K of elements, and inorganic, simple organic, and metallo-organic compounds. The two compilations are described separately below (Sections 1.1.6a. and 1.1.6b.).

A third continuing program is "Chemical Thermodynamics of Non-Ferrous Metallurgy" by J. I. Gerassimov, A. N. Krestovnikov, and A. S. Shakhov (Section 1.1.6c.).

1.1.6a. Thermodynamic Properties of Chemical Substances

Organization

The first edition of this compilation appeared in 1956 under the title "Thermodynamic Properties of Combustion Product Components." Its stated purpose was to aid in thermodynamic calculations of processes occurring at high temperatures. The next edition, described here, was published in 1962 under the new title "Thermodynamic Properties of Chemical Substances." Compilation of the values was done over a period of 10 years by collaborators in the Institute of Mineral Fuels (IGI) of the USSR Academy of Sciences and the USSR State Institute of Applied Chemistry (GIPKh) under the direction of V. P. Glushko and L. V. Gurvich. An associated research program in a number of institutions provided data missing from the literature.

Substances

Thermodynamic properties are given for the following elements and isotopes: O, H, D, T, He, Ne, Ar, Kr, Xe, F, Br, I, S, N, P, C, Si, Pb, Hg, Zr, B, Al, Be, Mg, Ca, Sr, Ba, Li, Na, K, Rb, and Cs, their oxides, hydrides, fluorides, chlorides, and nitrides in the solid (45 substances), liquid (44 substances), and gaseous (335 substances) phases, including monoatomic and diatomic ionized gases and electron gas. A first supplement recently completed gives properties for Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, and their oxides in the solid, liquid, and gaseous phases. The second and third supplements will consider compounds of alkaline and alkaline earth metals.

Properties

The following thermodynamic property values are given at selected temperatures for gases in the ideal state at 1 atmosphere pressure: Gibbs energy function $(G^\circ - H_0^\circ)/T$ or Φ_T^*, entropy S_T°, relative enthalpy $H_T^\circ - H_0^\circ$, heat of formation ΔH_f° or I_T°, equilibrium constant K_p and log K_p where K_p is the constant of dissociation or ionization. Values are given at 400 - 6,000°K at 100°-intervals and also at 293.15 and 298.15°K. For 22 substances, values up to 10,000°K are given at 200°-intervals and to 20,000°K at 500°-intervals. For compounds in the condensed phase, in addition to the above properties, values for heat capacity C_p° and vapor pressure P are given from 293.15°K to appropriate temperatures. Polynomial equations are given for the tabulated thermodynamic properties of gases.

Sources of Data

World literature; also data collected by the collaborating groups in the Soviet Union.

Critical Appraisal

Literature articles were carefully examined, and in many cases the experimental values were re-evaluated, enabling corrections to be made to the values to be included in the compilation. When necessary, recalculations were made to provide a system of self-consistent values. Estimates were made when experimental data were lacking. Volume I includes detailed discussions of the properties tabulated, the formulas used for calculation of their values, critical analyses and evaluation of the data found in the literature, and the bases for selection of the accepted values and their uncertainty limits. Errors in Gibbs energy function Φ_T^*, caused by uncertainties in values of molecular constants and the method of evaluation, are given for each gas. More than 4,000 references are cited by number in the body of the text.

Complete references, an author index with English equivalents of names, and a formula index to both Volumes I and II are included.

Use of Nomenclature, Symbols, and Units

Symbols, terminology, and values of constants used are those recommended by international organizations except when the recommendations differ materially from Soviet usage. All symbols, designations, and constants used are explained or defined in one of the appendixes. The values of all thermodynamic functions are expressed in calories per mole and calories per mole degree, and of equilibrium constants and vapor pressures in atmospheres.

Currency

The 1962 edition is a complete revision of the earlier edition and contains additional data, published from 1955 to 1961. Supplement I, the first of a number of supplements projected, contains mostly new information, although it does update a few tables from the earlier volume.

Format

The compilation consists of two bound volumes, 8 1/4" x 10 1/2". Volume I is largely descriptive, although it contains a number of short tables. Volume II consists entirely of tables, 380 of them presenting the thermodynamic properties of 335 substances. The elements are arranged in the order given under Substances which is similar to that of the Standard Order (Section 1.1.1. and Circular 500).

Publication and Distribution

Thermodynamic Properties of Chemical Substances, V. P. Glushko, et al., eds.

Vol. I, 1,164 pp., Vol. II, 916 pp., USSR Academy of Sciences, Moscow (1962), approximately $16.00. First supplement, in late 1966 or early 1967, also will be published by the USSR Academy of Sciences.

1.1.6b. Thermodynamic Constants of Substances

Organization

The program of compilation and publication of "Thermodynamic Constants of Substances" is sponsored by the USSR Academy of

Sciences under the direction of V. P. Glushko and V. A. Medvedev. A large group of specialists in several institutes has been enlisted to assist in the project. Two parts of a planned series of ten have appeared. Upon completion of the ten parts, the entire work incorporating new values and corrections will be issued in two volumes.

Substances

Thermal constants are given at 298.15°K for O, H, D, T, F, Cl, Br, I, At, ^{3}He, He, Ne, Ar, Kr, Xe, Rn, and their compounds (in all, 265 substances) in Part I and for S, Se, Te, Po, and their compounds in Part II. The compilation when completed will cover inorganic compounds of all elements, organic compounds containing not more than two carbon atoms, and metallo-organic compounds in which the organic group contains only one or two carbon atoms.

Properties

Thermodynamic property values: heat capacity $C_{p_{298.15°}}$, enthalpy $H^\circ_{298.15°} - H^\circ_0$; entropy $S^\circ_{298.15°}$; dissociation energy D_0; enthalpy of formation $\Delta Hf^\circ_{298.15°}$ and ΔHf°_0; Gibbs energy of formation $\Delta G^\circ f_{298.15°}$; enthalpy and entropy of polymorphic transformations, and of fusion, vaporization, and sublimation; temperature and vapor pressure at phase transformations; and critical temperature. Symmetry, structural type, and ionization potentials are given in the appendixes.

Sources of Data

World literature; also data collected or measured by thermodynamic specialists collaborating in the program.

Critical Appraisal

All values in the handbook are stated to be self-consistent, and an indication of the uncertainty is generally given. When necessary, values lacking in the literature were estimated. In some cases

special experimental investigations were carried out in Soviet institutions to supply needed data. A separate set of tables identifies the specific references for each value recorded by their numbers in a general list of references at the end of each part. There are 963 references listed in Part I and 718 in Part II.

Use of Nomenclature, Symbols, and Units

In general, the symbols, terminology, and units are those recommended by international organizations modified in part to accord with Soviet usage. The values of all thermodynamic constants are expressed in calories per mole and calories per mole degree, and vapor pressure is expressed in atmospheres. The symbols and abbreviations used are explained in the introduction.

Currency

Part I of the handbook was published in 1965 and Part II early in 1966. It is assumed that publication of the other parts will follow as scheduled (Part III in late 1966).

Format

The books, 8 1/4" x 10 1/2", have hard paperback covers. They consist almost entirely of tables. A long list of abbreviations for references cited is given in Part I and a short addendum to the list in Part II.

Publication and Distribution

Thermodynamic Constants of Substances, Handbook in 10 Parts, prepared under the scientific guidance of the USSR Academy of Sciences, V. P. Glushko, ed.

Part I, 1965, 146 pp., 72 kopecks ($1.75)*
Part II, 1966, 96 pp., 52 kopecks ($1.40)*

Published by the USSR Academy of Sciences, All-Union Institute of Scientific and Technological Information, Moscow.

* Available in the United States from Victor Kamkin, Inc., Bookstore, 1410 Columbia Rd., N.W., Washington, D.C. 20009.

1.1.6c. Chemical Thermodynamics in Nonferrous Metallurgy

The series of books, "Chemical Thermodynamics in Non-Ferrous Metallurgy," compiled by J. I. Gerassimov, A. N. Krestovnikov, and A. S. Shakhov and published in handbook form, is the outgrowth of two earlier publications, "Chemical Thermodynamics of Non-Ferrous Metallurgy" by Gerassimov and Krestovnikov in 1933, and "Thermodynamics of Physicochemical Properties of Rare Metals" by Krestovnikov and Shakhov in 1943.

Four volumes of the eight planned to encompass thermodynamic and physicochemical properties of industrially important nonferrous and rare metals have already been published. The authors' goal is to familiarize persons with thermodynamic methods and the calculations for pyrometallurgical processes, to present methods of calculation for thermodynamic properties of important nonferrous and rare metals, and to examine and compare existing literature of numerical data for the thermodynamics of nonferrous metallurgy and to examine the problems involved therein.

Substances

Important gaseous elements and compounds involved in nonferrous metallurgy, zinc, copper, lead, tin, silver, tungsten, molybdenum, titanium, zirconium, niobium, tantalum, aluminum, antimony, magnesium, nickel, bismuth, and cadmium, and their compounds to date.

Properties

Property values given include those for atomic volume, density, melting and boiling point, vapor pressure, specific and atomic heat capacity, enthalpy and entropy of formation and phase changes, Gibbs energy of formation, and enthalpy and Gibbs energy functions.

Sources of Data

World literature.

1.1.6c.

Critical Appraisal

Values reported are both experimental and calculated. When possible, recommended values are given. Lists of references are given for each chapter in Roman characters, except references to Russian publications. A number of the references are to other well-known compilations. The text is entirely in Russian but, because international symbols for properties and for chemical elements and compounds are used, equations and tables are easily understood by readers of other nationalities.

Currency

Although the references for data given in the early publications are quite old, there is a considerable number of references for data in the 1950's and some for data as late as 1962. The four volumes were published in 1960, 1961, 1963, and 1964.

Use of Nomenclature, Symbols, and Units

In general, the symbols, terminology, and units are those recommended by international organizations, modified in part to accord with Soviet usage. Volume I has a two-and-a-half-page table explaining symbols (in Russian).

Format

The books are attractively bound, 6" x 8 3/4". An English translation of Volume III is paperbound, 6 3/4" x 9 1/2".

Publication and Distribution

Chemical Thermodynamics in Non-Ferrous Metallurgy, J. I. Gerassimov, A. N. Krestovnikov, and A. S. Shakhov.

Vol. I: Theoretical Introduction, Thermodynamic Properties of Important Gases, Thermodynamics of Zinc and Its Important Compounds, 1960, 231 pp.

Vol. II: Thermodynamics of Copper, Lead, Tin, Silver, and Their Important Compounds, 1961, 263 pp.

Vol. III: Thermodynamics of Tungsten, Molybdenum, Titanium, Zirconium, Niobium, Tantalum, and Their Important Compounds, 1963, 283 pp.

Vol. IV: Thermodynamics of Aluminum, Antimony, Magnesium, Nickel, Bismuth, Cadmium, and Their Important Compounds, 1966, 428 pp.

Published by Metallurgical Publishing House, Moscow.
English translation of Vol. III published for the National Aeronautics and Space Administration and the National Science Foundation, Washington, D.C., by the Israel Program for Scientific Translations, available as NASA-TT-F-285 or CFSTI-TT-65-50111 from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Va. 22151.

1.1.7. SELECTED VALUES FOR THE THERMODYNAMIC PROPERTIES OF METALS AND ALLOYS: University of California, Berkeley

Organization

This project, started in 1955, is under the direction of Ralph Hultgren, Professor of Metallurgy, University of California, Berkeley. The work is carried out within the Inorganic Materials Research Division of the Lawrence Radiation Laboratory and the Department of Mineral Technology of the University. The sponsor of the compilation project is the U.S. Atomic Energy Commission with assistance from the American Iron and Steel Institute and, until recently, from a number of industrial firms. The project now operates as a participant in the National Standard Reference Data Program of the National Bureau of Standards. Unless otherwise stated, the material that follows refers to the book published in 1963 with the director as a coauthor (see Publication and Distribution).

Substances

All metallic elements and binary alloy systems for which published thermodynamic data have been found.

1.1.7.

Properties

Very complete thermodynamic data are given for both elements and alloys. For the elements, values for heat capacity, enthalpy (heat), entropy, and Gibbs energy (free energy) function relative to the standard states for both the condensed and gas phases at selected temperature intervals are tabulated. Frequently, empirical equations for calculation of enthalpy for solid and liquid phases and occasionally equations for heat capacity are included. Values for enthalpy and entropy of phase changes, for Gibbs energy and enthalpy of vaporization, and for vapor pressure are also given. For alloys, the integral quantities presented are enthalpy, Gibbs energy, entropy, excess Gibbs energy, and excess entropy of formation. Values for activities and activity coefficients and for partial molar thermodynamic quantities over a range of compositions (a, γ, $\Delta\overline{F}$, $\Delta\overline{F}^{xs}$, $\Delta\overline{H}$, $\Delta\overline{S}$, $\Delta\overline{S}^{xs}$) are also included as well as phase diagrams for most of the alloys.

Sources of Data

All available thermodynamic data for metallic elements and binary alloy systems published in journals or other compilations of critically evaluated data. To some extent, values are obtained by extrapolation or by calculation from values of other properties.

Critical Appraisal

A detailed introduction presents clearly the methodology and guidelines followed by the authors in their evaluation of data. The numerous graphical and analytic methods used to develop consistent and reliable values are discussed. Discrepancies between and within tables have been eliminated as far as possible. For each system reported, the survey of the literature and the evaluation of the data were conducted by a member of the staff under the supervision of one of the authors. The final evaluation was then reviewed and checked by at least three of the four authors before acceptance. The evaluation of each system is discussed so that the user of the tables is given the source and basis of selection and may, if he wishes, make his own study of the original data. When estimates and extrapolations are used to provide usable values where experimental ones have not been found, the values are given in parentheses. Uncertainties in tabulated values

are often recorded; when not recorded they may be estimated by the user of the tables from information given in the preliminary discussion of the system.

Use of Nomenclature, Symbols, Units, and Physical Constants

The values and units of the principal constants used (including both basic and derived constants) and, for comparison, the corresponding new values are tabulated. Most of the new values have been recommended by the Commission on Thermodynamics and Thermochemistry and the Commission on Data and Standards of the International Union of Pure and Applied Chemistry. Atomic weights are those of the chemical system (O = 16). Symbols, with the units in which they are expressed, are defined for the properties or conditions to which they refer. In the loose-leaf supplements beginning in October 1964, the units and constants used are those recommended by the Committee on Fundamental Constants of the National Academy of Sciences - National Research Council in 1963 and the atomic weights are those based on carbon-12.

Currency

Issuance of new and revised data sheets at intervals has kept the compilation up to date. In 1963, all data evaluated to about 1961-1962 were consolidated and published in book form. A new series of loose-leaf releases has been started.

Format

The interim publication form is the 8 1/2" x 11" loose-leaf sheet. The book, 7 1/4" x 9 3/4", appeared in 1963. It includes data for 63 elements and 168 alloy systems. For each system, Part I, Discussion, is followed by Part II, Tables (data and graphs). The values in the tables are at intervals close enough for linear interpolation. Data sources are given in the discussion, and complete references are listed in Part III. The pages are arranged alphabetically by chemical symbols and formulas; the metallic elements are in Chapter 2 and the alloy systems in Chapter 3. These chapters are photographic reproductions of the most recent data sheets at

the time of publication. A systems index by formula and an alphabetical author index for references to original data are provided.

Publication and Distribution

Selected Values for the Thermodynamic Properties of Metals and Alloys, Ralph Hultgren, Raymond L. Orr, Philip D. Anderson, and Kenneth K. Kelley, John Wiley & Sons, Inc., New York, N.Y. 10016, 1963, xi + 963 pp., $12.50.

Supplementary data sheets, having the same title as the book, are issued periodically. Requests for these sheets should be sent to Professor R. Hultgren, Department of Mineral Technology, University of California, Berkeley, Calif. 94720.

1.1.8. THERMOCHEMISTRY FOR STEELMAKING*

Organization

Under the sponsorship of the American Iron and Steel Institute, a program, directed by Professor J. F. Elliott, was established about eight years ago in the Department of Metallurgy of the Massachusetts Institute of Technology to collate, consolidate, and summarize in handbook form all available thermodynamic and physicochemical data for the substances and systems involved in steelmaking. The material is also relevant to the chemistry of many metallurgical systems at elevated temperatures. Although the original plan envisioned several volumes, most of the contemplated subject areas have been included in Volumes I and II. Compilation of related data is being continued by Professor Elliott under the sponsorship of the Office of Standard Reference Data, National Bureau of Standards.

Substances

Selected elements and compounds in their various states, phases and/or species that are involved in the chemistry and technology of

* The word "thermochemistry" is usually used in a restrictive sense to refer to properties of chemical reactions. Here it is used to include properties of both reacting and nonreacting systems for which the term "thermodynamics" or "chemical thermodynamics" is properly used.

steelmaking are treated in Volume I. The compounds include carbides, nitrides, oxides, phosphides, silicides, and sulfides. Volume II, in addition to elements and compounds, specifically treats binary and ternary iron alloys and solutions, complex oxide systems, and slags.

Properties

Thermodynamic properties are given for elements and compounds in their various states and phases, and for solutions. The properties include heat (enthalpy) and temperature of phase changes; heat capacity; enthalpy, entropy, and Gibbs energy function at 100-degree intervals; and enthalpy, Gibbs energy and log K_p of formation as appropriate. When available, the following properties are also given: density, thermal conductivity, electrical resistivity, total and spectral emissivity, viscosity, surface tension, vapor pressure, solubility (including that of gases), diffusion, activity, and activity coefficients. Phase diagrams, which take up approximately 30 percent of Volume II, include binary diagrams for elements, oxides, and iron solutions, and the effect of the addition of a second metallic element upon the solubility of graphite in iron.

Sources of Data

In Volume I, the authors list as major sources a number of existing compilations of data already critically evaluated by recognized experts in their fields, but the authors also used numerous reviews, journal articles and books, and some unpublished data. (The major sources include Bulletins 476, 477, and 542, listed in Section 1.1.5., and NBS Circular 500 described in Section 1.1.1. of this Survey: "Thermodynamic Properties of the Elements" by D. R. Stull and G. C. Sinke, and "Metallurgical Thermochemistry" by O. Kubaschewski and E. L. Evans.) For source material, Volume II depends much more on the open literature than on existing compilations.

Critical Appraisal

This publication may be classified as a handbook in which the aim has been to present up-to-date information mutually consistent with regard to base and reference states in forms useful in both the

laboratory and plant. Many of the diagrams and tables have appeared in other publications, but much new information from the literature, particularly in Volume II, is evaluated. The reasons for selection of revised values is not always indicated but references used are given, and short discussions precede the data for most systems. Readers are warned in cases where data have been extended by calculation or estimation to obtain values at high temperatures. This compilation is unique in that it includes useful thermodynamic properties of slag and metal solutions, interaction coefficients, and diffusion coefficients in melts. The authors point out that there are still enormous gaps in technical data related to steelmaking.

Use of Nomenclature, Symbols, Units, and Physical Constants

Most symbols and their units are given in the introduction of Volume I, Section 2, Thermochemical Properties of Selected Elements. Others are explained in the sections in which they appear. The Kelvin temperature scale is used in Volume I, but Fahrenheit and Celsius temperatures are plotted on the phase diagrams in Volume II. Weight percent is plotted linearly with atomic percent indicated at the top of the phase diagrams.

Currency

The time required for preparation of such a compilation, designed to fill a particular need, of necessity prevents the recorded values from being truly current. The authors recognized this fact and were meticulous in referencing their sources of data. The preface to Volume II is dated July 1963, but there are very few references later than 1960.

Format

The compilation consists of two bound volumes, 8 1/2" x 11". Each volume and some of the individual systems have a short introduction. The printing is excellent and the diagrams exceptionally clear. In addition to a detailed table of contents, each volume contains a comprehensive index. That of Volume I lists the elements and compounds under the properties recorded and not under their own names, that of Volume II is cumulative for the two volumes and lists topics,

titles of tables, substances, and systems of substances with properties under each.

Publication and Distribution

Thermochemistry for Steelmaking, Vol. I, J. F. Elliott and M. Gleiser, 1960, viii + 296 pp., $17.50.

Thermochemistry for Steelmaking, Vol. II, Thermodynamics and Transport Properties, J. F. Elliott, M. Gleiser, and V. Ramakrishna, 1963, xvi + 550 pp., (297-846), $25.00.

Published by Addison-Wesley Publishing Company, Inc., Reading, Mass. 01867.

1.1.9. THERMODYNAMIC FUNCTIONS OF GASES

Organization

The preparation of surveys of the thermodynamic properties of industrially important gases was started in 1948 under the supervision of the Thermodynamics Committee of the Mechanical Engineering Research Board of the Department of Scientific and Industrial Research (now the Department of Education and Science) of Great Britain. The late Dr. F. Din served as general editor of the series and contributed an introductory discussion, Thermodynamic Diagrams and Functions and Their Preparation, in Volume I, and the surveys on air, acetylene, and argon in Volume II and on nitrogen in Volume III.

Substances

Industrially important gases: ammonia, carbon dioxide, carbon monoxide, air, acetylene, ethylene, propane, argon, methane, nitrogen, and ethane.

Properties

Temperature - entropy diagrams, tabulated values for entropy, enthalpy, and volume for single phases and/or two phases in equilibrium,

specific heats at constant pressure and volume, and Joule-Thomson coefficients. Also given are physical properties including density, molecular volume, boiling point, triple point temperature and pressure, and critical constants.

Sources of Data

A comprehensive survey of all available data in the open literature for each gas considered.

Critical Appraisal

For each gas, the authors give (1) a critical and detailed survey of the existing data, (2) discussions of the calculation of the thermodynamic functions and of the construction of the temperature - entropy diagrams, (3) an appraisal of the accuracy of the compiled data, (4) a list of references to the open literature, and (5) tables of the thermodynamic functions. Short tables of the properties under discussion are included in the textual material. The quality of the evaluated data may vary from gas to gas because some details of treatment were left to individual authors. For example, the units used are consistent for an individual gas but are not consistent throughout the series. The temperature-entropy diagrams, on 6" x 10" pages, are too small for accurate interpolations. They are, however, also available in wall-sized charts.

Units

As indicated above, units vary. Enthalpies are given in calories per mole, kilocalories per kilogram, joules per mole, and joules per gram; volumes are sometimes expressed in cubic centimeters and sometimes in cubic decimeters. The International Steam Tables calorie (4.1868 absolute joules) is used.

Currency

The first two volumes, with data for eight gases, appeared in 1956, eight years after the surveys were initiated. Volume 3 appeared in 1965 at about the time of Dr. Din's untimely death. The series will

not be contined in the same form. A program with similar objectives, but aiming at higher quality, sponsored by the International Union of Pure and Applied Chemistry, has been started at Imperial College, London, England, and will lead to internationally recommended tables. It is under the general supervision of Professor D. M. Newitt, F.R.S., also associated with the earlier series, and is directed by Dr. Selby Angus.

Format

The surveys and compilations appear in bound books, 6" x 10". The pattern is the same for all gases, that is, textual material followed by tables of data. Each book has a table of contents but no complete index.

Publication and Distribution

Thermodynamic Functions of Gases, F. Din, ed., $12.50 per volume.
Vol. 1: Ammonia, Carbon Dioxide, Carbon Monoxide, 1956, viii + 175 pp.
Vol. 2: Air, Acetylene, Ethylene, Propane and Argon, 1956, vi + 201 pp.
Vol. 3: Methane, Nitrogen, Ethane, 1961, vi + 218 pp.

Temperature-entropy diagrams are available as wall charts at $3.00 each. Those for nitrogen and carbon monoxide are double charts, price $6.00.

Published by Butterworth & Co. (Publishers) Ltd., 88 Kingsway, London, W.C.2, England. Also available from Butterworth Inc., 7300 Pearl St., Washington, D.C. 20014.

1.2. THERMOPHYSICAL PROJECTS

1.2.1. THERMOPHYSICAL PROPERTIES OF CRYOGENIC MATERIALS: Cryogenic Data Center

Organization

The Cryogenic Data Center was established in 1958 in the Cryogenic Laboratory at the National Bureau of Standards (NBS), Boulder, Colo., and is directed by Victor J. Johnson. The Data Center has two major areas of activity, documentation and data evaluation. The latter activity includes the continuing correlation of data and the publication of tables of the thermophysical property values of materials used in low temperature applications. It is supervised by Richard B. Stewart with a staff of four or five professional and one or two clerical workers. Originally this project was sponsored by Wright Air Development Division (now Aeronautical Systems Division), U.S. Air Force. Later, the National Aeronautics and Space Administration became the project sponsor. The project now operates as a participant in the National Standard Reference Data Program of NBS. Close contact is maintained with related experimental programs in the Cryogenic Laboratory.

Substances

Cryogenic fluids and selected solids. The fluids include helium, hydrogen (particularly parahydrogen), neon, nitrogen, oxygen, carbon monoxide, and binary mixtures of some of them; and to a limited extent, air, fluorine, and methane. Solids of interest in cryogenic engineering for which property values have been reported include metals, ferrous and nonferrous alloys, and a few inorganic and organic compounds.

Properties

All thermophysical properties in the temperature range from near absolute zero to ambient temperatures are included in the program with emphasis on the properties useful in engineering applications

to cryogenic systems. The properties include density, expansivity, thermal conductivity, specific heat, enthalpy, phase transition heats, phase equilibria (such as vapor pressure, melting point, critical point), dielectric constants, absorption, surface tension, viscosity, compressibility factor, entropy, PVT values, vapor-liquid concentrations of binary mixtures and velocity of sound in the medium for fluids; and thermal expansion, thermal conductivity, specific heat and enthalpy of solids. Temperature - entropy, pressure - enthalpy, and similar relations are published in chart form.

Sources of Data

Original papers from the world literature, available unpublished data, and original calculations.

Critical Appraisal

The objectives of the compilation tasks are to present critically evaluated and internally consistent sets of data over wide ranges of temperature and pressure. In the preparation of the tables, related data are compared and evaluated on appropriate theoretical and statistical bases. "Best values" are selected from the data and appropriate theoretical models are determined. This study provides the basis for prediction of additional values necessary to fill the gaps in the ranges of pressure and temperature needed and determination of the uncertainties in the resulting tables of values.

Use of Nomenclature, Symbols, Units, and Physical Constants

Wherever practical, the units used are those of the International System, as adopted by the 11th General Conference on Weights and Measures in 1960. In some cases deviations from the International System of units are used to increase the utility of the tables for engineers. The symbols and terminology used for physical quantities are in general compatible with proposed international standards. A number of the technical notes are issued in both English and metric units.

1.2.1.

Currency

Since the issuance of the Compendium (see below), new or revised data on one or several substances have been issued mainly as NBS Technical Notes and journal articles. Plans include issuance of more comprehensive compilations as NBS Monographs.

Format

"A Compendium of the Properties of Materials at Low Temperatures, Phase I" was published as paperbound but easily separated 8 1/8" x 10 5/8" sheets punched for standard three-hole binders, and the sheets for Phase II are similar. The NBS Technical Notes are paperbound booklets, 8" x 10 1/2". The thermodynamic charts are issued separately on 17" x 22" or 8 1/2" x 11" sheets.

Publication and Distribution

A Compendium of the Properties of Materials at Low Temperatures, V. J. Johnson, ed.

Phase I, Part I, Properties of Fluids, July 1960, 489 pp., WADD Technical Report 60-56, Part I (PB-171-618), $6.00.*

Phase I, Part II, Properties of Solids, Oct. 1960, 330 pp., WADD Technical Report 60-56, Part II (PB-171-619), $4.00.*

Phase I, Part III, Bibliography of References (cross-indexed), Oct. 1960, 161 pp., WADD Technical Report 60-56, Part III (PB-171-620), $3.00.*

Phase II, R. B. Stewart and V. J. Johnson, eds., Dec. 1961, 501 pp., WADD Technical Report 60-56, Part IV (AD-272-769), $8.10.*

A limited number of the thermodynamic charts and other publications of the Cryogenic Data Center are available from the Center, NBS, Boulder, Colo. Price of the 17" x 22" charts is 25 cents, and the 8 1/2" x 11" charts, 10 cents. Prices of the other publications are quite varied.

Interested, qualified persons may write to the Director of the Cryogenic Data Center requesting that their names be placed on a mailing list to receive announcements and notification of availability and cost of new publications.

Technical Notes, Monographs, and many journal articles are listed in "Publications of the National Bureau of Standards," supplements of which are issued periodically and may be obtained from NBS. Compilations of thermodynamic properties issued as Technical Notes and Monographs include the following:

The Thermodynamic Properties of Nitrogen From 64 to 300°K Between 0.1 and 200 Atmospheres, Thomas R. Strobridge, NBS Technical Note 129, (PB-161 630), Jan. 1962, 85 pp., $2.25.*

The Thermodynamic Properties of Helium From 3 to 300°K Between 0.5 and 100 Atmospheres, Douglas B. Mann, NBS Technical Note 154, Jan. 1962, 95 pp., 50 cents.†

Thermodynamic Property Values for Gaseous and Liquid Carbon Monoxide From 70 to 300°K With Pressures to 300 Atmospheres, J. G. Hust and R. B. Stewart, NBS Technical Note 202, Nov. 1963, 109 pp., 60 cents.†

Thermodynamic and Related Properties of Parahydrogen From the Triple Point to 100°K at Pressures to 340 Atmospheres, H. M. Roder, L. A. Weber, and R. D. Goodwin, NBS Monograph 94, Aug. 1965, 112 pp., 75 cents.†

* Available from the Clearinghouse for Federal Scientific and Technical Information, U.S. Department of Commerce, Springfield, Va. 22151 (the PB- and AD-numbers are given when known, to facilitate ordering the reports from the Clearinghouse).
† Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

1.2.2. THERMOPHYSICAL PROPERTIES RESEARCH CENTER

Organization

The Thermophysical Properties Research Center (TPRC), established in 1957 at the School of Mechanical Engineering, Purdue University, Lafayette, Ind., became a separate department in the Schools of Engineering in 1962. The areas of activity of TPRC include scientific documentation, generation of data tables, and research. A major aim of TPRC is the correlation and evaluation of data and the publication of tables. The professional staff of more than 25 members, consisting of chemists, physicists, and chemical and mechanical engineers, carries on a supporting research program. The original sponsors were 26 industrial, nonprofit, and governmental research organizations. The present primary support for the compilations program is received from the Air Force Materials Labora-

tory, Research and Technology Division, Air Force Systems Command, U.S. Air Force, Wright-Patterson Air Force Base, Ohio, and the Office of Standard Reference Data of the National Bureau of Standards. Dr. Y. S. Touloukian has been director of TPRC since its inception.

Substances

The data correlation part of the TPRC program covers metallic elements and their alloys in solid, liquid, and gaseous states (Volume I); nonmetallic elements, compounds, and mixtures that exist in the liquid or gaseous state at 25°C and one atmosphere pressure (NTP) (Volume II); and nonmetallic elements, compounds, and mixtures that exist in the solid state at NTP (Volume III). Substances are selected on a priority basis for given properties. Early emphasis was on thermal conductivities of metals.

Properties

The aim is to cover all transport and thermodynamic properties needed in heat and mass transfer calculations. Seven properties were selected for initial coverage, namely, thermal conductivity, viscosity, thermal radiative properties, thermal diffusivity, specific heat, diffusion coefficient, and Prandtl number. The first four properties were given priority. Values for a given property are reported in the same chapter in each volume, i.e., thermal conductivity property values are given in Chapter 1, viscosity data in Chapter 2, data for thermal radiative properties in Chapter 3, thermal diffusivity data in Chapter 4, and specific heat data in Chapter 5. To date, portions of Chapter 1 have been issued for all three volumes, portions of Chapter 2 for Volume II only; emittance data of Chapter 3 have been issued for Volumes I and III and reflectance data for Volume I; portions of Chapter 4 have been issued for Volumes I and III and of Chapter 5 for all three volumes. Data are being compiled for thermal absorptance and transmittance. For each of the radiative properties, namely, emittance, reflectance, absorptance, and transmittance, data are being processed for hemispheral, normal, and angular observations both total and spectral. Irrespective of its physical state, all physical properties of a given substance are given in the volume corresponding to the physical state of the substance at normal temperature and pressure.

Sources of Data

World literature; foreign and English language abstracting services; governmental, academic, and industrial research reports; masters and doctoral theses from accredited colleges and universities; and cooperative arrangements with major research laboratories in the United States and abroad.

Critical Appraisal

The stated aims are (1) to produce, whenever possible, an internally consistent set of "most probable" or "recommended" values of a particular property of a material as of a given date; (2) to supplement experimental data by semiempirical correlation methods when such methods are justified; and (3) by use of statistical thermodynamics, to generate tables of transport properties when experimental values for such properties are not available. These aims are met by the critical evaluation, analysis, and correlation of existing data and the calculation, when possible, of values to fill gaps in the available data. In Volumes I and III, tables or graphs or both for all experimental values recorded are given. Since December 1962, recommended values for those substances for which they have been selected have been given on a separate chart and table. Estimated errors in recorded values are also indicated. In Volume II, only recommended values are tabulated and they are accompanied by graphic "departure plots," which show the percentage difference between the experimental and tabulated values. The "Specification Table" gives for each curve the literature reference number, experimental method used, year of measurement, temperature range, reported errors, specimen designation, and composition of the material in weight percent. The pertinent constants used in the equations for the calculations of thermal conductivity are given above the tabular results for each element.

Use of Nomenclature, Symbols, Units, and Physical Constants

Policies concerning symbols and units, etc., take into account the dual orientation to engineering and pure science and are those accepted or recommended by international organizations such as the International Organization for Standardization. Symbols, units, and conversion factors used are given in the introductory material of each chapter.

1.2.2.

Currency

Revised and new sheets are issued semiannually. Supplementary sheets giving recommended values are being issued as rapidly as possible. As of June 1966, thermal conductivity values had been reported for 642 substances including all metals and a number of alloys, 38 nonmetallic substances in both the gaseous and liquid states, 14 in the gaseous state only, 2 in the liquid state only, and 552 in the solid state. The data are maintained on a current basis in all three volumes. Work on viscosity has been held in abeyance for the past two years to give priority to specific heat studies. All materials on which thermal diffusivity data are available are covered and the data are maintained on a current basis. Specific heat values were issued for the first time for all three volumes in June 1966. The total valid sheets are summarized under Publication and Distribution.

Format

Loose-leaf 11" x 17" data sheets are printed on one side. Data are presented in both tabular and graphic form. As indicated under Substances, the data are issued in three volumes divided into chapters according to property. Each material studied is assigned a serial number, and all figures and tables pertaining to that material bear the assigned number, thus making insertion of new sheets possible without destroying the sequence of the following sheets. Tables of recommended value are designated by an R after the serial number. Literature references are given at the end of each chapter. The introductory material includes a table of contents and sections on general information and generation of recommended values, a discussion with explanations of symbols and units used, and an alphabetical directory of materials.

Publication and Distribution

Thermophysical Properties Research Center Data Book. Issued as loose-leaf sheets.

Vol. I: Metallic Elements and Their Alloys.

Vol II: Nonmetallic Elements, Compounds and Mixtures (In Liquid and Gaseous States at Normal Temperature and Pressure).

Vol. III: Nonmetallic Elements, Compounds and Mixtures (In the Solid State at Normal Temperature and Pressure).

Summary of Valid Data Sheets as of June 30, 1966

	Thermal Conductivity	Viscosity	Radiative Properties	Thermal Diffusivity	Specific Heat
Pages	1512	123	486	204	208
Substances	642[a]	53	116	73	119

[a] Includes 210 materials in the composite tables of Chapter 1 in Vols. I and III.

Data sheets are sold on a subscription basis at 10 cents per sheet. Academic institutions and organizations authorized by the sponsor may obtain the data sheets gratis. Imprinted buckram flexipost binders, $20.00 per volume.

Order from Thermophysical Properties Research Center, Purdue University, Research Park, 2595 Yeager Rd., West Lafayette, Ind. 47906.

Note: TPRC has prepared two volumes, each in three parts, of the "Retrieval Guide to Thermophysical Properties Research Literature," which make possible a search of the contents of world journals, reports, and books for references to articles containing thermophysical data on practically all substances. Vol. III, in preparation, will complete coverage of the world literature from 1920 through June 1964 for the seven selected groups of properties.

Retrieval Guide to Thermophysical Properties Research Literature, Y. S. Touloukian, ed.
Vol. I, Books 1, 2, and 3, 1960, $150,00; Volume II, Books 1, 2, and 3, 1964, $150.00; McGraw-Hill Book Company, 330 W. 42nd St., New York, N.Y. 10036.

1.2.3. THERMOPHYSICAL PROPERTIES OF SOLID MATERIALS

This project, described in the first edition of this survey with the title "Directory of Continuing Numerical Data Projects" was carried out at the IIT Research Institute (then the Armour Research Foundation of Illinois Institute of Technology) under contract with the Air Force Materials Laboratory, Wright-Patterson Air Force Base, Ohio. It was terminated with the publication, in 1958, of a five-volume report, "Thermophysical Properties of Solid Materials," WADC

Technical Report No. 58-476. The report has since been published by the Macmillan Company from whom the five volumes may be obtained. Substances for which properties are included are elements, alloys, ceramics, cermets, and intermetallics melting above 1,000° F, and polymeric and composite materials of any melting temperature. Much of the subject matter in these volumes is being upgraded in quality and brought up-to-date by the Thermophysical Properties Research Center under contract with the Air Force Materials Laboratory. (See Section 1.2.2. for a description of this center.)

Publication and Distribution

Handbook of Thermophysical Properties of Solid Materials, A. Goldsmith, T. E. Waterman, and H. J. Hirschorn, revised edition, 1961 (8 1/2" x 11 1/4"), The Macmillan Co., 60 Fifth Ave., New York, N.Y. 10011, $90.00 per set.

Vol. I: Elements, vi + 752 pp.

Vol. II: Alloys, vi + 1,270 pp.

Vol. III: Ceramics, vi + 1,162 pp.

Vol. IV: Cermets, Intermetallics, Polymerics and Composites, vi + 798 pp.

Vol. V: Appendix (includes materials, author indexes, and a list of references), 286 pp.

1.3. PHYSICOCHEMICAL PROJECTS

1.3.1. CHEMICAL KINETICS DATA PROJECT

Organization

This project, no longer active, was established in the 1940's at Princeton University under the direction of the late Professor N. Thon and supported jointly by the University, the National Bureau of Standards (NBS), and the National Research Council (NRC). Charles H. Stauffer became project director in 1954 and continued the work,

first at Worcester Polytechnic Institute and after 1958 at St. Lawrence University, Canton, N.Y. Administrative supervision was provided by the Division of Chemistry and Chemical Technology of NRC and technical supervision by the NRC Subcommittee on Kinetics of Chemical Reactions. Before 1961 financial support came mainly from the Office of Ordnance Research, Department of the Army, and from 1961 to 1963, jointly from the National Science Foundation, the U.S. Atomic Energy Commission, the Office of Naval Research, the Army Research Office (Durham), and NBS. All publication was through NBS. The staff included members of the chemistry department of St. Lawrence University and expert collaborators in various universities. The project was terminated in June 1963, and the final publication appeared in July 1964. The files of the project have been transferred to the recently established Chemical Kinetics Information Center at NBS. This center is supported by the Department of Defense Advanced Research Projects Agency and the NBS Office of Standard Reference Data.

Substances

Homogeneous inorganic and organic reactions in the gaseous, liquid, and solid phases.

Properties

The publications include values for the following: rate constants (from the "defined mass-action law"); frequency factors; and heats, energies, and entropies of activation. Where no rate constant could be derived from the available data, empirical rates were sometimes given.

Sources of Data

Most, but not all the pertinent journals in the world literature. References mentioned in secondary articles were examined.

1.3.1.

Critical Appraisal

Stress is laid throughout on experimentally ascertained facts. Kinetics measurements by their nature are often not very precise, but values were averaged or selected when possible. The solvent (often one of the reactants), the amount of addend (catalyst), temperature, and concentration are specified. When ambiguity exists, a statement is made to indicate the exact reaction or reactant for which the rate is given. Closely agreeing data were averaged and are underlined in the tables. Less concordant data are often given side by side, the range of variability serving as a guide to the reproducibility of the rate of reaction. Additional information pertinent to the evaluation is sometimes given in a Comments section. In Circular 510 three indexes are included: a subject index based on type of reaction; an alphabetical index of reaction types; and an alphabetical index of the classes of compounds involved in the reactions published. Literature references used or mentioned in Comments are appended to each table. Monograph 34 has only a subject index.

Use of Nomenclature, Symbols, Units, and Physical Constants

A systematic effort was made to have all results conform to a uniform mode of presentation based on time in seconds, concentration in moles per liter, and temperature in degrees Centigrade; rate constants are those based on natural logarithms.

Currency

Complete and current coverage of the whole domain of homogeneous reaction kinetics was not possible with the staff available. By concentrating on selected types of reaction, currency was reasonably well maintained in some areas. Omissions from and additions to the earlier tables were included in new supplements as they appeared. Literature references through 1960 were included, and termination dates for coverage were given on each sheet.

Format

The tables are issued in the form of 8 7/8" x 11 3/8" punched sheets temporarily assembled under a paper cover which may be removed for loose-leaf filing. This arrangement permits supplementary sheets to be filed in their proper places in the compilation. 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 order of increasing complexity of the key reactant. Each table is designated by a number that refers to the type of reaction, phase of reaction, and type of substances involved. For tables requiring more than one page, the table number is repeated and pages numbered.

Publication and Distribution

Tables of Chemical Kinetics, Homogeneous Reactions, NBS Circular 510, 1951, xxiv + 732 pp. (out of print).

Tables of Chemical Kinetics, Homogeneous Reactions, NBS Circular 510, Supplement 1, 1956, xiv + 422 pp. (out of print).

Alphabetical Index to Tables of Chemical Kinetics, Homogeneous Reactions, NBS Circular 510, Supplement 2, 1960, iv + 37 pp., 35 cents.

Tables of Chemical Kinetics, Homogeneous Reactions, Supplementary Tables, To Accompany Circular 510 and Supplements 1 and 2, NBS Monograph 34, 1961, $2.75.

Tables of Chemical Kinetics, Homogeneous Reactions, Supplementary Tables, NBS Monograph 34, Vol. 2, 1964, $2.00.

Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

1.3.2. PHASE DIAGRAMS FOR CERAMISTS

Organization

The American Ceramic Society and National Bureau of Standards (NBS) sponsor this compilation activity. Early compilers were

1.3.2.

F. P. Hall, Herbert Insley, and H. F. McMurdie. Authors of the 1964 compilation were E. M. Levin, Carl R. Robbins, and H. F. McMurdie, of NBS. Other members of the NBS staff and of the American Ceramic Society contribute phase diagrams, make suggestions, and note errors. The society also provides editorial assistance. Compilations are now financed from a revolving fund created by the Board of Trustees of the society from sales of previous issues.

Substances

Systems selected because of their interest to ceramists, specifically metal-oxygen and metal oxide systems, systems with oxygen-containing radicals, systems containing halides, sulfides, cyanides, and water, alone and with other substances, and fused salt systems. Borides, carbides, and silicides are not included.

Properties

Simple and complex phase diagrams for one-, two-, three-, and multicomponent systems. For some systems, multidiagrams show phase relations at various temperatures, and for others, isotherms, isofracts, temperature - composition projections, compatibility relations, and base systems of tetrahedra are given. Melting points of metallic oxides, molecular weights of oxides, and 1961 atomic weights of the elements are given in separate tables.

Sources of Data

World literature (including Russian).

Critical Appraisal

Although the selection of diagrams to be included was still somewhat arbitrary, the authors were more critical in the 1964 edition than in previous ones. Usually, when several diagrams existed for a given system, the compilers selected the one they deemed best. However, occasionally the authors included several diagrams representative of current interpretation or composite diagrams constructed from the work of several investigators. Sometimes figure reproductions were

made from tracings of edited enlargements of the original diagrams to improve legibility and uniformity of statement. Although many diagrams are too small to permit values to be read with accuracy, diagrams of partial systems, such as a high corner of a ternary system or an enlargement of a complicated portion of a system, increase the legibility.

The introductory material includes the following: a comparison of three temperature scales that have been used since 1914, a general discussion of phase diagrams that contains a glossary of terms, a statement of the phase rule and its limitations, interpretations of the different types of diagrams, a discussion of experimental methods of phase equilibrium determinations at high temperatures, and an enlarged selected and annotated bibliography that covers theory, interpretation, methods and techniques, mathematical treatment, thermodynamic calculations, silicate chemistry, special collections of phase diagrams, and phase diagrams in related fields.

Use of Nomenclature, Symbols, and Units

Temperatures are in degrees Celsius, but it is not always apparent whether the scale is the Geophysical Laboratory Temperature Scale of 1914 or the International Temperature Scale of 1927 or 1948. Compositions are given in weight percentage unless otherwise stated.

Currency

The first compilation of this project appeared in the "Journal of the American Ceramic Society" in 1933. Supplements or revisions were published in the same journal in 1938, 1947, and 1949. Compilations in book form were issued in 1956, 1959, and the latest in 1964, with a literature cutoff date of early 1962, though a few later diagrams are included. It supersedes all previous publications of the series and brings the textual material up to date.

Format

Two complete compilations with a supplement to each were published in the "Journal of the American Ceramic Society" between 1933 and 1949. A third complete compilation in 1956 and its supplement,

Part II, in 1959 appeared in book form (7 7/8" x 10 7/8"). The 1964 compilation, also in book form, is slightly larger, 8 1/2" x 11 1/2". The diagrams are grouped according to system composition and within each group are listed in order of increasing complexity. They are sometimes accompanied by explanatory notes, and complete references are given below each diagram. An author index and a system index are included.

Publication and Distribution

Phase Diagrams for Ceramists, E. M. Levin, H. F. McMurdie, and F. P. Hall, 1956, 286 pp. (811 phase diagrams).

Phase Diagrams for Ceramists, Part II, E. M. Levin and H. F. McMurdie, 1959, 153 pp. (462 phase diagrams).

Phase Diagrams for Ceramists, E. M. Levin, C. R. Robbins, and H. F. McMurdie (7th compilation) 1964, 601 pp. (2,064 phase diagrams), $18.00 (discount to members).

Phase Equilibrium Diagrams of Oxide Systems, revised and redrawn by E. F. Osborn and A. Muan. (Ten 19" x 23" plates for three-oxide systems containing SiO_2, four of them for oxide phases in equilibrium with metallic iron. Reproductions of these plates appear in the 1964 compilation.)

Published by The American Ceramic Society, 4055 N. High St., Columbus, Ohio 43214.

1.3.3. CONSTITUTION OF BINARY ALLOYS

Organization

The "Constitution of Binary Alloys" by Max Hansen with the cooperation of Kurt Anderko was published in 1958 as a revised edition of Hansen's "Der Aufbau der Zweistofflegierungen" which was published in 1936 and which served for over 20 years as an outstanding reference work. The 1936 edition was so widely in demand that an offset printing of the German edition was made in the early 1940's and distributed in the United States. Compilation of the 1958 edition was carried out at the IIT Research Institute (then the Armour Research Foundation of Illinois Institute of Technology) under the sponsorship

of the U.S. Air Force, Wright-Patterson Air Force Base, Ohio. The "Constitution of Binary Alloys, First Supplement," published in 1965, was also compiled at the IIT Research Institute under the same sponsorship. Both Dr. Hansen and Dr. Anderko had returned to Germany, and the work on the supplement was done under the direction of Rodney P. Elliott who has since moved to the University of Cincinnati. Dr. Elliott still serves as consultant for the project.

Substances

More than 1,700 binary systems in the 1965 edition and more than 2,000 in the combined 1958 and 1965 editions. The systems are mostly alloys, although borides, hydrides, oxides, chalcogenides, and phosphides are included.

Properties

Phase diagrams are given for many systems. Properties and their values, which are discussed concisely, include solubility, eutectic point, melting point, crystal structure, and cell dimensions.

Sources of Data

All available literature. For the 1965 edition, references were found principally by searching Chemical Abstracts, Metallurgical Abstracts, and Review of Metal Literature, but some specialized abstract bulletins, bibliographies, reviews, and monographs were used.

Critical Appraisal

The authors analyzed and evaluated all the information found. Their conclusions are not always discussed in detail but are in most cases incorporated in composite diagrams based upon their evaluations of the data. If a diagram is that of an individual author, it is so designated. The text and diagrams should be used together; uncertainties in the data or hypothetical phase relations are indicated by dashed lines. The Supplement is a true supplement and not a revised edition of Hansen's compilation. Its table of contents is a cumulative listing

of systems contained in both editions and indicates whether a diagram is given. Also, titles in the Supplement indicate whether the system was included in the 1958 edition. The reader is cautioned not to use a diagram without the text nor the material in the Supplement without reference to the previous review if such exists. Factors for use in the interconversion of atomic and weight percent for each system are given in both editions, but the directions and tables needed to use them are in the 1958 edition only. Thus possession of the 1958 edition is a necessity for full use of the Supplement.

Use of Units and Constants

The phase diagrams are plotted with a linear atomic percent scale, but a nonlinear weight percent scale is also given.

Currency

The 1958 edition covered the literature up to the spring of 1955, with some data published in 1956 and 1957. The 1965 edition reviews literature pertinent to binary systems published through December 1961. Work is in progress on the preparation of a second supplement covering the literature published from 1962 through 1964.

Format

Book form, 6" x 9". The systems are alphabetically ordered by chemical symbols. Tables of some physical properties and structural data of the elements are included in the appendixes to both the 1958 edition and the 1965 Supplement. The 1958 edition also has a table on crystal-structure types according to "Strukturbericht," and conversion tables for temperatures and for atomic and weight percentages.

Publication and Distribution

Constitution of Binary Alloys, M. Hansen and K. Anderko, 1958, xix + 1,305 pp., $39.50.

Constitution of Binary Alloys, First Supplement, R. P. Elliott, 1965, xxxii + 877 pp., $35.00.

Published by McGraw-Hill Book Company, 330 W. 42nd St., New York, N.Y. 10036.

1.3.4. STABILITY CONSTANTS OF METAL-ION COMPLEXES

Organization

The first edition of "Stability Constants of Metal-Ion Complexes, with Solubility Products of Inorganic Substances," was compiled by J. Bjerrum of the Københavns Universitet, Copenhagen, G. Schwarzenbach of Eidgenössische Technische Hochschule, Zürich, and L. G. Sillén, Kungliga Tekniska Högskolan, Stockholm, under the auspices of the Commission of Equilibrium Data of the International Union of Pure and Applied Chemistry. It was published in two parts by The Chemical Society, London; Part I: Organic Ligands, Special Publication No. 6, 1957, and Part II: Inorganic Ligands, Special Publication No. 7, 1958. The second edition, published in 1964, appeared as Special Publication No. 17, in one volume: Section I—Inorganic Ligands, compiled by Professor Sillén, and Section II—Organic Ligands, compiled by Professor A. E. Martell, IIT Research Institute, Chicago.

Substances

All soluble complexes for which data are available, and many solid compounds of both organic and inorganic ligands with metallic ions. (All elements except the so-called noble gases are included as metal ions.) The hydrogen ion is considered as a metal and the electron and the hydroxyl ion as ligands.

Properties

Equilibrium constants are given, expressed as logarithms to the base 10. They include those for reactions of ligands with "metal" ions, for acidic and basic reactions both stepwise and cumulative, for redox and special reactions, and for solubility constants. The minimum number of constants necessary to represent the author's results are given. Enthalpy and entropy changes are often recorded. Some equilibrium constants for liquid-liquid distribution are given.

1.3.4.

Sources of Data

Primarily world literature, but a few private communications.

Critical Appraisal

All available values are recorded. A value considered doubtful by the author is indicated by the sign ?. one considered doubtful by the compiler, by the sign (?). No attempt has been made to select best values. The compilers state that the sign (?) could have been used more frequently in a critical compilation and that its absence should not be construed as a recommendation of the value given, nor its presence as a reproach. The method of measurement, temperature, medium, and coded references are given for each entry with a list of complete references following each table.

Use of Symbols and Units

The units for concentration are generally in moles per liter. The abbreviations and symbols used to describe the media in which the measurements are made are explained in the introductory material and are consistent with IUPAC recommendations.

Currency

The 1957 edition (Organic) included all available data published to the end of 1955; the 1958 edition (Inorganic) included data to the end of 1956 and some from 1957. The 1964 edition includes all available data published to the end of 1960, some that appeared in 1961-1963, and a few data omitted in the first edition.

Format

The data are published in book form, 7 1/4" x 10", in six-column tables, the form and content of which are adequately described in an introductory section, "How to Use the Tables." Briefly, in the Inorganic section both the ligands and the metal ions of each ligand - metal pair are arranged in an order based upon the subgroups of the

Periodic Table. In the Organic section the ligands are arranged according to Beilstein's system and the metal ions alphabetically by their symbols. An index of inorganic ligands and an index of organic ligands are arranged alphabetically by names and an index of metals is arranged alphabetically by symbols.

Publication and Distribution

Stability Constants of Metal-Ion Complexes, with Solubility Products of Inorganic Substances, compiled by Jannik Bjerrum, Gerold Schwarzenbach, and Lars Gunnar Sillén.

Part I: Organic Ligands, Special Publication No. 6, The Chemical Society, London, 1957, xvi + 105 pp. (out of print).

Part 2: Inorganic Ligands with Solubility Products of Inorganic Substances, Special Publication No. 7, The Chemical Society, London, 1958, xvi + 131 pp. (out of print).

Stability Constants of Metal-Ion Complexes, Section I: Inorganic Ligands, compiled by Lars Gunnar Sillén; Section II: Organic Ligands, compiled by Arthur E. Martell; Special Publication No. 17, The Chemical Society, London, 1964, xviii + 754 pp., $23.00 (actually a 2nd edition of above with a slightly changed title).

Available from the General Secretary, The Chemical Society, Burlington House, London, W.1., England.

1.3.5. SEIDELL'S SOLUBILITIES OF INORGANIC, METAL-ORGANIC, AND ORGANIC COMPOUNDS

Organization

Atherton Seidell's famous series of compilations of solubilities has been appearing at 6- to 12-year intervals since 1907 when the first edition consisting of 353 pages of tables appeared. The second edition, with more than twice as many pages as the first, was published in 1919; a supplement to the second edition in 1928; and the two volumes of the third edition in 1940 and 1941. In 1951 W. F. Linke joined Dr. Seidell, A. W. Francis, and R. G. Bates in the preparation of a 1,254-page supplement to the third edition which appeared in 1952. The

first volume of the fourth edition, under the authorship of W. F. Linke, was published in 1958 and the second volume in 1965. Volume III, "Solubilities of Organic Compounds," is in preparation under the authorship of Alan F. Clifford and Gerald W. Dulaney. In 1943 Dr. Seidell assigned the copyright to the American Chemical Society (ACS), which assumed responsibility for publication of later volumes.

Substances

Elements and inorganic, metal-organic, and organic compounds for which solubilities are found in the literature. Volume I of the fourth edition covers the elements and their inorganic compounds from argon (A) through iridium (Ir) arranged alphabetically by their chemical symbols. Volume II covers the solubilities of the elements and compounds from potassium (K) through zirconium (Zr).

Properties

Solubilities in water; in aqueous solutions of acids, bases, salts with and without a common ion, and organic compounds; in anhydrous organic and inorganic solvents; in high temperature mixtures (salt melts). Phase diagrams are given for some systems. References, but no values, are given for the solubility of gases in metals, and solubility products are given sometimes.

Sources of Data

In the earlier editions, most of the material was gathered through direct searching of original journals. Because of the rapid increase in the number of original sources, Chemical Abstracts was used as the starting point for locating new information for the fourth edition. Original publications were then obtained for extraction of data.

Critical Appraisal

The tables of data were prepared by combining, comparing, and evaluating results of various authors. Closely agreeing results were sometimes averaged; clearly unreliable results were omitted.

If there was no clear choice between conflicting sets of data, both sets were included. Introductory statements evaluate the data found in the references given. Because of the diversity of sources, investigators, and methodology, uniformity in the quality of data cannot be expected. The source of the data recorded is generally indicated, and an author index gives complete references by year.

Currency

In the fourth edition, the plan was for each volume to cover the literature up to the year preceding its publication. Volume I, published in 1958 (manuscript completed in 1957), covered the literature through 1956. The publication of Volume II was delayed. It was released in February 1966 and covers the literature through the early 1960's. Publication of the Organic volume in 1968 or soon thereafter will be followed as soon as practical by a fifth edition.

Units

Solubilities are given in different units, but those used for each substance are clearly indicated.

Format

Publication is in hard-cover books, 6" × 9". The offset printing is clear but in the indexes suffers from overreduction. Elements are listed alphabetically by their chemical symbols, and their compounds are listed alphabetically according to the chemical symbols of their anions or radicals. In complex systems of more than one solute, data are placed under the solute that is alphabetically first but are indexed under each substance. Volume II of the fourth edition contains cumulative indexes covering Volumes I and II for subjects and literature cited (formerly author index).

Publication and Distribution

Before 1943, D. Van Nostrand Company, Inc., published this compilation. After 1943 when the copyright was assigned to ACS, the books were published by ACS but continued to be distributed by Van Nostrand

until mid-1965. Since that time, they have been both published and distributed by ACS.

Solubilities of Inorganic and Organic Compounds, Supplement to the 3rd edition, 4th printing, 1953, iv + 1,698 pp. (out of print).

Solubilities of Organic Compounds, A. Seidell, Vol. II, 3rd edition, 4th printing, 1953, vi + 926 pp. (out of print).

Solubilities of Inorganic and Organic Compounds, Supplement to the 3rd edition, A. Seidell and W. F. Linke with sections by A. W. Francis and R. G. Bates, 1952, iv + 1,254 pp. (out of print).

Solubilities of Inorganic and Metal Organic Compounds, A Compilation of Solubility Data from the Periodical Literature, A. Seidell, 4th edition, Vol. I, W. F. Linke, 1958, iv + 1,287 pp., $32.50.

Solubilities of Inorganic and Metal Organic Compounds, A Compilation of Solubility Data from the Periodical Literature, A. Seidell, 4th edition, Vol. II, W. F. Linke, 1965, iv + 1,914 pp., $32.50.

Available from American Chemical Society, Special Issues Sales, 1155 Sixteenth St., N.W., Washington, D.C. 20036.

1.4. INDEXES

1.4.1. CONSOLIDATED INDEX OF SELECTED PROPERTY VALUES: PHYSICAL CHEMISTRY AND THERMODYNAMICS

Prepared by the Office of Critical Tables. A key to the contents of six compilations* that present critically evaluated numerical property values. Publication 976, National Academy of Sciences - National Research Council Printing and Publishing Office, 2101 Constitution Ave., N.W., Washington, D.C. 20418, 1962, xxiii + 274 pp., cloth-bound, $6.00.

* Five of these compilations are discussed in this survey as Projects 1.1.1., 1.1.2., 1.1.3., 1.1.5., and 1.1.7. The sixth, a single compilation, is Thermodynamic Properties of the Elements, D. R. Stull and G. C. Sinke, v + 234 pp., American Chemical Society Advances in Chemistry Series No. 18, $5.00.

2
Crystallographic, Mineralogical, and Other Solid State Projects

2.1. CRYSTALLOGRAPHIC PROJECTS

2.1.1. CRYSTAL DATA

Organization

The publication "Crystal Data" is the work of many crystallographers who helped in collecting and assembling data, in making calculations, and in editing. The first edition, published in 1954 as Memoir 60 of the Geological Society of America, with the subtitle "Classification of Substances by Space Groups and Their Identification from Cell Dimensions," consisted of two parts: Part I: Systematic Tables—Classification of Crystalline Substances by Space Groups, written by Werner Nowacki, University of Berne, Switzerland; and Part II: Determinative Tables—Identification of Crystalline Substances from Cell Dimensions, written by J. D. H. Donnay, the Johns Hopkins University, Baltimore, Md., with the collaboration of Gabrielle Donnay, U.S. Geological Survey, Washington, D.C., and many assistants. The second edition (1963) is a revision of Part II only, with

2.1.1.

J. D. H. Donnay as general editor and Gabrielle Donnay as assistant editor. Coeditors were E. G. Cox, University of Leeds, and Agricultural Research Council, London, for inorganic compounds; Olga Kennard, National Institute for Medical Research, London, and the University Chemical Laboratory, Cambridge, England, for organic compounds; and Murray Vernon King, Massachusetts General Hospital, Boston, Mass., for proteins (Appendix I). The 1963 edition appeared as Monograph 5 of the American Crystallographic Association (ACA). Cooperation and encouragement for the work was received from the International Union of Crystallography, its Commission on Crystallographic Data, related national commissions in Japan and the Soviet Union, and ACA, particularly its Crystal Data and Publication committees. Financial support for the second edition was received from the National Science Foundation in the United States, and the Institute of Physics (U.K.). Preparation of the third edition is continuing under a grant from the National Bureau of Standards (NBS) through the Office of Standard Reference Data.

Substances

Elements, inorganic and organic compounds of molecular weight less than 2,000 with the exception of the proteins. Only a few alloys are included in the second edition because, in the opinion of the authors, alloys are adequately covered in "A Handbook of Lattice Spacings and Structures of Metals and Alloys" by W. B. Pearson, published by Pergamon Press (see section 2.1.5.).

Properties

Crystallographic data resulting mainly from x-ray and electron-diffraction measurements are presented. Cell dimensions, axial ratios (determinative numbers), space group, the number (Z) of formula units per cell, and measured and calculated specific gravities are given for each substance if they are available. For many substances, auxiliary properties such as melting point, color, pleochroism, twinning, cleavage, and crystal habit are given. Under Structure, the structual type is given for compounds in the older literature. For recently studied compounds an indication is made as to whether the structure has been determined and if so whether it is qualitative or quantitative (atomic coordinates determined). Optical

properties such as index of refraction, optic axial angle, and orientation are given for a number of compounds. Space-group criteria are given in Appendix II.

The first edition of "Crystal Data" was the first compilation to list single crystal data in a manner useful for determinative purposes. The method used was dependent upon the choice of a cell by arbitrary rules based on metric considerations. The Delaunay-reduced cell used in the first edition was replaced in the second edition by the Bravais-reduced cell (defined by the shortest three translations).

Sources of Data

Many of the data for the first edition were obtained from secondary sources such as Strukturbericht, Structure Reports, Chemical Abstracts, Mineralological Abstracts, and Bulletins analytiques (now Bulletins signalétiques). Although references were obtained from these sources for the second edition, original papers were checked, so revised entries are from primary references, except in a few cases where the original paper was not available. Secondary sources, when used, are clearly indicated. Some prepublication data are included. In the words of one reviewer, "This work is by far the most comprehensive guide to the sources of crystal data."

Critical Appraisal

All new data (1951 and later) were processed and checked by either the Leeds or the London office and all data (new as well as old) were transformed, whenever required. Many crystallographers provided corrections to errors in the first edition. The data sheets were further edited and errors eliminated in the Baltimore office. Data from more than one source are often given. The Introduction to Part II (second edition), Determinative Tables, adequately describes the methods of compilation and presentation of the data.

Use of Nomenclature, Symbols, Units, and Physical Constants

Since Parts I and II were prepared independently, conventions adopted for presentation of data were not the same in the two parts, though within each part uniformity was attempted. The cubic cell edges are given in ångström units, having been transformed from kX

units when necessary. For noncubic substances, unless otherwise stated the date of the reference indicates whether the unit is kX or ångström, those before 1949 being in kX units and those dated 1949 and later in ångström units. No attempt has been made to obtain uniformity of nomenclature, the chemical name usually being given as it appears in the literature. Both chemical and mineral names are often given and both are listed in the index.

Currency

Part I of the first edition covers the literature to mid-1948 and Part II to the end of 1951. The cutoff date for the second edition (Part II) was December 31, 1960, but the 1960 data included are incomplete. A Single Crystal Date File is maintained with the data recorded on cards, enabling the data to be revised as new values are obtained. Thus, material for the third edition was being collected even during preparation of the manuscript for the second edition.

Format

Data are presented in tables and lists. In Part I (first edition) the main table lists substances by space groups subdivided into seven categories based on composition. Substances are characterized by name and stoichiometric formula, the classification being alphabetical, first by name, then by formula. References are included. Statistical results obtained from the main table are presented in six tables. Compounds in each crystal system are listed by increasing determinative number (axial ratio of the Bravais-reduced cell or the cubic cell edge). Formula and name indexes are given (in the first edition, cumulative for the two parts). References for Part I (first edition) are given at the end of Part I and for Part II (both editions) in the individual entries. The second edition includes as Appendix I, "Protein Crystal Data" and as Appendix II, "Tables of Space-group Criteria." Appendix I in the main follows the same type of format as that used in the determinative tables. The modifications are explained in the introduction to the appendix.

Production of the third edition by use of the linofilm machine controlled by the output of a digital computer is being planned under the financial responsibility of NBS, with joint sponsorship of ACA.

Publication and Distribution

Crystal Data, Classification of Substances by Space Groups and their Identification from Cell Dimensions, J. D. H. Donnay and Werner Nowacki, Memoir 60 of the Geological Society of America, 1954, ix + 719 pp., Geological Society of America, 419 W. 117 St., New York, N.Y. 10027 (out of print).

Crystal Data, Determinative Tables, second edition, J. D. H. Donnay, General Editor; Gabrielle Donnay, Assistant Editor; E. G. Cox, Inorganic Compounds; Olga Kennard, Organic Compounds; Murray Vernon King, Proteins; Monograph 5 of the American Crystallographic Association, 1963, x + 1,302 pp., $20.00. Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pa. 15238.

Crystal Data, Systematic Tables, second edition, Werner Nowacki (in preparation).

2.1.2. CRYSTAL STRUCTURES

Organization

The author of "Crystal Structures" is Ralph W. G. Wyckoff, University of Arizona, Tucson, Ariz. The first edition of this five-volume reference work, including several supplements, appeared in loose-leaf form during the period 1948 to 1960. In response to a need, an amplified and updated version of the original work is being published in book form. Three volumes of this second edition have appeared.

Substances

Elements, inorganic compounds of the structures RX, RX_2, R_mX_n, $R(MX_2)_n$, $R_n(MX_3)_p$, $R_n(MX_4)_p$, $R_x(MX_m)_y$, hydrates, ammoniates, silicates, and miscellaneous types (one chapter), and organic compounds including aliphatic, aromatic, alicyclic, and heterocyclic compounds and carbohydrates, discussed in that order. Volume I of the second edition covers elements, and compounds RX and RX_2. Volume II covers compounds R_nX_m (n and m interchanged in second edition), $R(MX_2)_n$, and $R_n(MX_3)_p$. Volume III covers compounds $R_x(MX_4)_y$, $R_x(M_nX_p)_y$, hydrates, and ammoniates.

2.1.2.

Properties

Type of crystal, unit cell dimensions, axial angles, unit cell structure, interatomic distances (coordinates). The content of the second edition is restricted to those determinations that define the position of most, if not all, the atoms in a crystal. Diagrams and packing drawings are given for most of the structures.

Sources of Data

Primary articles from world literature.

Critical Appraisal

The cell dimensions given are those the author considers the best currently available. No estimate of the accuracy of spacing measurements is included.

Use of Nomenclature, Symbols, Units, and Physical Constants

The terminology used conforms to that of (1) Internationale Tabellen zur Bestimmung von Kristallstrukturen, (2) the more recent International Tables for X-ray Crystallography, and (3) "Krystallsysteme und Krystallstruktur" and "Theorie der Kristallstruktur" by A. Schoenflies.

Currency

During the years of publication of the loose-leaf sheets, individual chapters were revised by issuance of supplements about every five years. To give the same coverage, plans for the second edition call for the publication of one volume per year for five years and then the revision of one volume per year in the same order. The bibliography of Volume I lists complete references by year of publication from 1914 through 1961, that of Volume II through 1962, and that of Volume III through 1963.

Format

Publication of the first edition was in loose-leaf sheets (7 3/4" x 9 3/4") for which special post binders are available. The compilation was divided into chapters with the material in each chapter divided into text, tables, illustrations, and bibliography. The volumes of the second edition are published in book form, 6 1/4" x 9 1/4". The chapters follow the order of the first edition. As in the first edition, each chapter is provided with a master table (Bibliography Table) which lists the crystals described and gives the paragraph reference of each description and literature references to the bibliography. Each volume contains a name index and a formula index.

Publication and Distribution

Crystal Structures, first edition

Section I: Chapters I to VIII, 1948, 378 pp., $13.50.
Section II: Chapters VIII-X, XIII, 1951, 509 pp., $17.00.
Section III: Chapters XIV, XV, Organic Index, 1953, 465 pp., $25.00.
Section IV: Chapters XI and XII, 1957, 261 pp., $8.00.
Supplement I: Additions to Chapters II to VII, 1951, 143 pp., $5.00.
Supplement II: Additions to Chapter XIII, 1953, 85 pp., $8.50.
Supplement III: Additions to Chapters II to VIII, 1958, 311 pp., $20.00.
Supplement IV: Additions to Chapters IX, X, XIII-XV, 1959, 509 pp., $22.00.
Supplement V: Additions to Chapters II to XV, Indexes, 1960, 513 pp., $26.50.

Binders for loose-leaf material are available together with a plan for insertion. Binders are provided free of charge with Sections I, II, and III. For balance of material, the charge is $4.00 each.

Directions for filing give:

Vol. I: Chapters I-IV.
Vol. II: Chapters V-VIII.
Vol. III: Chapters IX-XII, Inorganic Formula, Mineralogical Name Index.
Vol. IV: Chapter XIII.
Vol. V: Chapters XIV and XV, Index to Organic Compounds.

Supplements are filed with chapters. Complete set with necessary binders, $153.50.

Crystal Structures, second edition

Vol. I: Chapters I-IV, 1963, 467 pp., $17.50.
Vol. II: Chapters V-VII, 1964, 588 pp., $24.00.
Vol. III: Chapters VIII-X, 1965, 981 pp., $27.50.

Interscience Publishers, a division of John Wiley & Sons, New York, London, Sydney.

2.1.3. POWDER DIFFRACTION FILE: Joint Committee on Chemical Analysis by Powder Diffraction Methods

Organization

This activity is carried out under the joint auspices of the American Society for Testing and Materials (ASTM), the American Crystallographic Association, the Institute of Physics (U.K.), and the National Association of Corrosion Engineers. It is administered by ASTM, who, with the National Academy of Sciences - National Research Council, started the project in 1941. The aims of the committee, composed of representatives of the sponsoring organization and invited research scientists, are to collect, edit, and publish powder diffraction data with convenient indexes and to advance the technique by which these diffraction data can be used for chemical identification. The present chairman of the committee is W. L. Fink. The current editor is J. V. Smith, Department of Geophysical Sciences, The University of Chicago; associate editors are L. G. Berry, Queen's University, Ontario, Canada, for minerals; Benjamin Post, Polytechnic Institute of Brooklyn, Brooklyn, N.Y., for inorganic and organic substances; Sigmund Weissmann, Rutgers—The State University of New Jersey, New Brunswick, N.J., for metals and alloys; and Mrs. Mary B. Lotz, the bibliographer. The committee finances research associateships at the National Bureau of Standards (NBS) where, in the Constitution and Microstructure Section, needed measurements are made.

Substances

Solid materials, organic and inorganic, of interest to science and industry. Metals and alloys are included.

Properties

Powder patterns in terms of interplanar spacings, relative intensities, and Miller indices are recorded, with the interplanar spacings corresponding to the three strongest lines in the diffraction pattern given special prominence. Also given are crystallographic systems, space groups, lattice parameters, interaxial angles, indices of refraction, density, melting point and color, operating characteristics such as wavelength of x rays used and type of filter, number of formula units per structural unit, and molecular and semistructural formulas (when available).

Sources of Data

Patterns are submitted by groups in the United States (particularly those at NBS and those working under editors Smith, Berry, Post, and Weissmann), Great Britain, the Netherlands, Norway, Israel, and Japan. Data from the literature and from individual investigators are also included.

Critical Appraisal

The quality of data is continually being upgraded as the result of elimination of errors and careful editing of new patterns in their fields by the associate editors. In 1957, the data in Sets 1 - 5 were critically reviewed and new cards issued, marked "unchanged," "minor correction," or "major correction," as appropriate. A star in the upper right-hand corner indicates data of high reliability, a circle, low reliability. A critical review of the data in Sets 6 - 10 was begun in 1965 preparatory to issuance in book form. Comments on and reported errors in the File have been given in supplements to the File since 1964.

Currency

Each year a new set of data is added to the File. It contains new patterns and revisions of old ones. Set 16 (1966) contains data for 300 organic and 900 inorganic substances. The indexes also are brought up to date annually.

2.1.3.

Format

The x-ray powder diffraction patterns are presented on 3" × 5" plain cards for manual operation, 4" × 6" Keysort cards, and standard IBM cards. The cards may be arranged in order of the d-values of the strongest three lines, but are usually filed in order of issue. Revised sets 1 - 5 are also issued as clothbound books, one for inorganic and one for organic substances. Three cards are reproduced on a page. Sets 6 - 10 in book form are in preparation.

There are now three types of cumulative indexes, two in book form and one on optical coincidence cards. The "Index to the Powder Diffraction File" is issued in two volumes, Organic and Inorganic. Each has a numerical (Hanawalt) index and an alphabetical (Davey) index. In the Hanawalt index the use of three entries per compound permits each of the three strongest lines to be given the lead position in one entry. The Davey Inorganic Index lists chemical names in one section and mineral names in another. In the Organic Index, one section lists names, the other, formulas according to the Chemical Abstracts or Hill System in which CH is followed by all other symbols in alphabetical order.

The "Fink Index to the Powder Diffraction File" (Inorganic only) was introduced in 1963. It lists the eight strongest lines but no intensities. Eight entries arranged in cyclic permutations of d-values are given for each substance. This index is useful not only for identification of substances by means of x-ray powder diffraction but also by electron diffraction. The Matthews Coordinate Index (Termatrex cards) includes standard, supplementary, and negative element cards. Negative Line cards became available in 1964. Data obtained from patterns measured at NBS are published separately by them in paper-covered booklets.

Publication and Distribution

Sixteen sets (approximately 13,000 cards) of the Powder Diffraction File (formerly known as the X-Ray Powder Data File) have been published by ASTM. They may be purchased separately in any of the available card forms.

Prices of File and Indexes

X-Ray Powder Diffraction Data File (PD-1), 16 Sets

Sets	Indexes	Cards		
		Plain ($)	Keysort ($)	IBM ($)
1 - 16	Organic	715	1,125	300
	Inorganic	1,280	1,855	
16 only	Organic	60	95	25
	Inorganic	140	220	

Book Form

1 - 5	Organic	25
	Inorganic	45
	Both	60

6 - 10 available in early 1967

X-Ray Powder Diffraction Data File—Computer Tapes

IBM magnetic tapes are available, containing in card image form all d-spacings and relative intensities with comments as given in the ASTM X-Ray Powder Diffraction File (sets 1 - 16). Write to ASTM for details and prices.

Indexes

Organic,* PDIS-16o, $15,00.
Inorganic,* PDIS-16i, $20.00; both, $30.00.
Inorganic (Fink),* PDIS-16f, $15.00.
Matthews Coordinate Index
Termatrex Cards, 16 sets, $675.00.
Negative-Line Cards, $185.00.
(Special rate for updating sets.)

* The appropriate index books and the Phase Designation of Alloys are furnished without charge with Set 16 plain and Keysort cards.

Orders should be sent to the American Society for Testing and Materials, Diffraction Data Sales, 1916 Race St., Philadelphia, Pa. 19103.

Related Publications

List of Alloy Phase Designations of the X-Ray Diffraction Data File, Sections 1-12, PD-2, S. Weissmann, 63 pp., $2.00. Supplied gratis with Set 15, Inorganic Section, available separately from ASTM.

Standard X-Ray Diffraction Powder Patterns, issued as NBS Circular 539, Vols. 1-10, 1953-1960 and as NBS Monograph 25, 1962 —. Section 1, 1962, 56 pp., 40 cents; Section 2, 1963, 46 pp., 35 cents; Section 3, 1964, 64 pp., 40 cents; Section 4, 1966, 83 pp., 55 cents.

Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

2.1.4. STRUCTURE REPORTS

Organization

"Structure Reports," an annual collection of abstracts of a special type, is a continuation and replacement of "Strukturbericht," which was published in seven volumes from 1913 through 1939. Work on "Structure Reports" began in 1949 under the guidance of the Commission on Structure Reports of the International Union of Crystallography. From 1949 through 1959, the reports were published under the general editorship of A. J. C. Wilson, University College, Cardiff, Great Britain, with section editors for metals, inorganic compounds, and organic compounds. In 1960, W. B. Pearson, National Research Council, Ottawa, Canada, became general editor. 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 (the Netherlands Organization for Pure Scientific Research), and other organizations in these three countries. The volumes issued since 1957 are sold at prices designed to recover the cost of production.

Substances

Metals, inorganic and organic crystalline compounds.

Properties

Unit cell dimensions, space groups, atomic positions and parameters, and interatomic and intermolecular distances are given. The data

presented are derived primarily from x-ray diffraction measurements. Only material of structural interest is extracted from papers, which may contain material of great interest from other viewpoints. Papers containing data obtained by electron diffraction, neutron diffraction, and nuclear magnetic resonance studies are reported when of structural interest. Papers of these types in Russian, Japanese, and other journals not readily available have been included more freely than those in easily accessible sources.

Sources of Data

Research papers in world literature, collected by reporters in several countries.

Critical Appraisal

This publication is intended as a source of precise information on all determinations of crystal structures, providing critical reports rather than abstracts. It aims at giving complete structural information from the papers reported so that no further reference is necessary to the papers themselves. The minimum criterion for preparing a report is generally that the paper contain the determination of a unit cell or a more accurate determination of a unit cell previously reported. Detailed assessments of each structure are made and critical comments are inserted by the reporters and editors when necessary. A structural report may even be longer than the paper itself through the addition of interatomic distances or other information calculated by the reporters from the data in the paper. Limits of error are often indicated and very doubtful last digits are enclosed in parentheses.

Currency

"Structure Reports" covers the period from 1940 (Volume 8) onward and thus forms a continuous series with the last volume of "Strukturbericht" (Volume VII). The latest volume published (1965) is 23 for 1959. The currency is still very poor, despite the fact that there are now teams of editors working on all years up to 1965. The editor estimates that the best currency that could be achieved is a lag of three to four years behind the period covered. The field covered is

now somewhat restricted so that much of the fringe material dealing with cold work, epitaxy, etc., is being omitted. With the increase in the number of papers being published, which is expected to continue, this restriction seems necessary in order to limit the size of the yearly volumes.

Format

"Structure Reports" is published in book form. Data are presented in tables, diagrams, and text. The volumes are divided into three main sections: Metals, Inorganic Compounds, and Organic Compounds. In the Metals section the arrangement is mainly alphabetical. Substances in the other sections appear roughly in the order of increasing complexity of composition. In each volume there are subject, formula, and author indexes and since 1955 an index of carbon compounds. Volume 14 contains a few supplementary reports for the period 1940-1950, but is mainly a cumulative index for Volumes 8 through 13. Most volumes have a corrigenda for previous volumes.

Publication and Distribution

Structure Reports, Vols. 8 - 16 and Vol. 18, A. J. C. Wilson, General Editor; Vol. 17 and Vols. 19 - 23, W. B. Pearson, General Editor; published for the International Union of Crystallography by N. V. A. Oosthoek's Uitgevers, Mij, Utrecht, the Netherlands. Agent in the U.S.—Polycrystal Book Service, Box 11567, Pittsburgh, Pa. 15238.

The years covered, year published, and price of each volume are as follows:

Volume	Years Covered	Year Published	Price	
			Dutch florin	$
8	1940-1941	1956	80	22.50
9	1942-1944	1955	70	19.50
10	1945-1946	1953	55	15.50
11	1947-1948	1951	100	28.00
12	1949	1952	70	19.50
13	1950	1954	100	28.00
14[a]	1940-1950	1959	35	10.00
15	1951	1957	110	31.00

[a] Index.

Volume	Years Covered	Year Published	Price	
			Dutch florin	$
16	1952	1959	120	33.50
17	1953	1963	125	35.00
18	1954	1961	120	33.50
19	1955	1963	100	28.00
20	1956	1963	100	28.00
21	1957	1964	100	28.00
22	1958	In preparation	. . .	. . .
23	1959	1965	120	33.50

Note: A new reprint of "Strukturbericht," Supplement to Zeitschrift für Kristallographie, forerunner to "Structure Reports," was published in 1965 by the Johnson Reprint Corporation, 111 Fifth Ave., New York, N.Y. 10003, and Johnson Reprint Company, Ltd., Berkeley Square House, London, W.1 , England. Orders may be sent to them or to Polycrystal Book Service (address page 70).

Vols. 1-7, Leipzig, 1913/1928-1939, clothbound, $140.00 per set; paper-bound, $120.00 per set.

Vols. 1-3, 1913/1928-1935, paper-bound, $20.00 per volume; clothbound, $23.00 per volume.

Vols. 4-7, 1936-1939, paper-bound, $15.00 per volume; clothbound, $18.00 per volume.

2.1.5. A HANDBOOK OF LATTICE SPACINGS AND STRUCTURES OF METALS AND ALLOYS

Organization

The first volume of the above handbook, compiled by W. B. Pearson, National Research Council, Ottawa, Canada, was published in 1958. The second volume is in preparation. The object of the publication is to provide in a single volume an appraisal and record of all structural work on metals and alloys.

Substances

Metals and binary, ternary, and a few higher alloys, including intermetallic phases of carbides, hydrides, nitrides, and oxides.

2.1.5.

Properties

Structural details; crystallographic data for Strukturbericht types; atomic lattice parameters and variations of the latter with composition in solid solution ranges and with temperature; also densities and expansion coefficients. The second volume will include a classification of structures of elements and alloy phases according to the Bravais lattice and number of atoms per unit cell. From the data given, known structures of any alloy phase can be drawn up and interatomic distances calculated. In some cases it may be necessary to obtain the coordinates of the appropriate point-sets from Volume I of "International Tables for X-ray Crystallography" (see Section 2.1.6.).

Sources of Data

Research papers in world literature.

Critical Appraisal

A critical selection is made in order to present only the most accurate data for all systems. In making the selection, weight has been given to metal purity, knowledge of exact composition and equilibrium temperature, and reliability of the x ray or other means of investigation. Each system is discussed to the extent justified by available data. Complete references are included.

Use of Nomenclature, Symbols, Units, and Physical Constants

In Volume I, settings of all orthorhombic and monoclinic crystals were generally transformed to the Standard Settings given in the International Tables for X-Ray Crystallography, and the particular author's use of kX or ångström units was generally maintained. In Volume II, the settings were not changed so often, and the data are given in ångström units. If units are in doubt, the fact is noted in text.

Currency

Volume I, published in 1958, reviewed all available structural work on metals and alloys through 1955 and some through 1956. Volume II will review practically all the work on alloys to the end of 1963, much of the work to the end of 1964, and some through 1965. The tables listing structural data for alloy phases will be entirely revised to include all data in Volumes I and II.

Format

Publication is in book form, 6 1/4" x 10". Volume I is divided into two parts. Part I, consisting of five chapters (75 pages) is largely textual, although 45 figures and 5 short tables are included. Part II, consisting of seven chapters (960 pages), reviews data and presents them in text, tables, and diagrams. The systems are arranged alphabetically by chemical symbols. The content of Volume II (1,446 pages) corresponds to Part II of Volume I.

Publication and Distribution

A Handbook of Lattice Spacings and Structures of Metals and Alloys, No. 4 of Pergamon Press series of monographs on Metal Physics and Physical Metallurgy. W. B. Pearson, Pergamon Press, Ltd., Headington Hill Hall, Oxford, England, also London, Edinburgh, New York, Paris, and Frankfurt, 1958, x + 1,044 pp., $38.00.
Volume II scheduled for publication in 1966.

2.1.6. INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

Organization

The three volumes of tables in this series were planned by the International Union of Crystallography (IUCr) to bring up to date the former Internationale Tabellen zur Bestimmung von Kristallstrukturen (International Tables for the Determination of Crystal Structures) published in 1935. They have been prepared under the direction of an editorial committee of the IUCr with Dame Kathleen Lonsdale as general editor. Individual crystallographers from many countries have contributed to the compilation and in Volumes II and III have

authored entire sections or subsections. Publication of Volume I, and indirectly of Volumes II and III, was made possible by the generous financial help of UNESCO and the National Academy of Sciences - National Research Council (U.S.). The Netherlands Organization for Pure Research (Z.W.O.), the N. V. Philips' Gloeilampenfabrieken, Eindhoven, the Netherlands, and the University College, London, provided support for Volume III in the form of secretarial and editorial assistance, or in allowing an editor to spend part of his time on this compilation.

Properties

Volume I, Symmetry Groups, presents tables, explanations, and diagrams for crystal lattices, point-group symmetry, and space-group symmetry. Volume II, Mathematical Tables, contains information of a mathematical nature, such as tables of functions, formulas, and geometrical diagrams. Volume III, Physical and Chemical Tables, is concerned with the processes involved in the x-ray study of crystals. Tables of many types of data and descriptive material useful to the student of crystal structures are included in each of the following sections: X Rays and Their Interaction with Crystals; Measurement and Interpretation of Intensities; Interatomic and Interionic Distances; and Texture and Line-Broadening Analysis—Small Angle Scattering. Among the tables, those on interatomic and interionic distances are noteworthy.

Sources of Data

As indicated above, tables of data and descriptive material have been supplied by expert crystallographers from many countries. The extensive bibliographies reveal use on a selective basis of both the primary literature and existing compilations.

Critical Appraisal

Methods of calculating tabulated values are discussed, and references are cited when possible. In the words of one of the authors, "Detailed acknowledgement of sources for such a compilation is almost impossible since many tabulations are classical and have been handed down through generations of texts." Necessary symbols are explained, and

the difficulty of maintaining complete consistency is admitted. Although the main text is in English, a Dictionary of Crystallographic Terms for each volume is given in English, French, German, Russian, and Spanish. Terms other than strictly crystallographic ones are also defined if needed for complete understanding of the text.

Currency

The plan to revise the 1935 tables was formulated in 1946. Volume I of the present tables appeared in 1952, Volume II in 1959, and Volume III in 1962. The Commission on International Tables of IUCr has under consideration a revision of the tables.

Format

The binding and printing of these 8 1/2" x 11" volumes is of the usual fine quality from the Kynoch Press. Each volume has a detailed table of contents, and Volume III has a cumulative general subject index.

Publication and Distribution

International Tables for X-Ray Crystallography, Kathleen Lonsdale, general editor.

Vol. I: Symmetry Groups, Norman F. M. Henry and Kathleen Lonsdale, eds., 1952, xii + 558 pp., £5.5.0. ($14.70).

Vol. II: Mathematical Tables, John S. Kasper and Kathleen Lonsdale, eds., 1959, xviii + 444 pp., £5.15.0. ($16.10).

Vol. III: Physical and Chemical Tables, Caroline H. MacGillavry and Gerard D. Rieck, eds., 1962, xvi + 362 pp., £5.15.0. ($16.10).

Published for the International Union of Crystallography by the Kynoch Press, Witton, Birmingham 6, England. Also available from Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pa. 15238. (Special prices to members of the American Crystallographic Association for their personal use.)

2.1.7. 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 crystallographers in the Department of Mineralogy of the University Museum at Oxford. Numerous cooperating individuals in Great Britain, the Netherlands, 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, composed of representatives of the Government, learned societies, universities, and industrial firms. Dr. A. E. J. Vickers was chairman of the committee from 1945 until his death in 1956, when he was succeeded by J. Wren-Lewis. Financial and material help have come from academic, governmental, and industrial organizations in England and the Netherlands. Editors for Volumes I and II were Dr. Mary W. Porter and the late R. C. Spiller, both of Oxford University, and for Volume III, Dr. Porter and L. W. Codd of Imperial Chemical Industries.

Substances

Volume I gives crystal descriptions of 2,991 compounds belonging to the tetragonal, hexagonal, trigonal, and orthorhombic systems; Volume II gives descriptions of 3,572 monoclinic substances and Volume III, descriptions of 831 substances in the anorthic system. Most of the substances are those described in Groth's five-volume "Chemische Krystallographie" (1906-1919).

Properties

The Barker system is based on the use of a small number of interfacial angles chosen for indexing purposes: a single angle for tetragonal, hexagonal, and trigonal crystals; three angles for orthorhombic crystals; five for monoclinic; and six for anorthic. In addition to the classification angles, axial ratios, symmetry, forms, habit, physical properties (cleavage, color, specific gravity, melting

point, etc.), optical properties (including refractive indexes), transformations, and in some cases the strongest three lines in the x-ray powder diffraction pattern are 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."

Critical Appraisal

Calculations for Volumes I and II were made independently by two workers and checked by one of the editors. The authors of Volume III state that so many errors of axial ratios, axial angles, and calculated angles for the anorthic system were found in Groth that individual notes and corrections could not be made. Corrected values were obtained by use of a computer. Adaptation of the Barker method to anorthic crystals was much more difficult than for the systems described in Volumes I and II. The rules finally agreed upon were lengthy but were shortened by use of an atlas of configurations developed by Dr. M. H. Hey of the British Museum of Natural History, and a table of configurations developed by the University of Groningen (the Netherlands) workers under Professor P. Terpstra. By use of these aids and with a Ferranti mercury computer the tedious calculations for anorthic crystals were completed. However, the machine, though able to detect errors in computed angles, could not correct errors in experimental data taken from Groth, which may not have been correctly transferred from the original source.

Use of Nomenclature, Symbols, Units, and Physical Constants

Accepted crystallographic symbolism has been used; technical terms, particularly those peculiar to the Barker technique, are explained.

Currency

It is unfortunate that so long a time was required to produce the three volumes. The publication covers essentially old literature,

mainly that of Groth, with few references to later data, so that the user has no assurance that the substance to be identified will be found in the index. Other recent compilations include many more substances.

Format

Part 1 of all three volumes has the subtitle "Introduction and Tables." Part 2 of Volumes I and III and Parts 2 and 3 of Volume II are entitled "Crystal Descriptions," with the compounds arranged in the same order as in Groth's "Chemische Krystallographie." Part 2 of Volume III also includes the "Atlas of Configurations." References to the data sources are given in the crystal descriptions.

Publication and Distribution

The Barker Index of Crystals, A Method for the Identification of Crystalline Substances.

Vol. I, Crystals of the Tetragonal, Hexagonal, Trigonal and Orthorhombic Systems, M. W. Porter and R. C. Spiller, 1951.
Part 1: Introduction and Tables, ix + 350 pp., £1.10.0. net ($4.20).
Part 2: Crystal Descriptions, x + 1,086 pp., £4.10.0. net ($12.60).
The two parts—£6.0.0. net ($16.80).

Vol. II, Crystals of the Monoclinic System, M. W. Porter and R. C. Spiller, 1956.
Part 1: Introduction and Tables, v + 383 pp.
Part 2: Crystal Descriptions, M.1 to M.1800, viii + 760 pp.
Part 3: Crystal Descriptions, M.1801 to M.3572, viii + 688 pp.
The three parts—£10.0.0. net ($28.00).

Vol. III, Crystals of the Anorthic System, M. W. Porter and L. W. Codd, 1964.
Part 1: Introduction and Tables, vi + 50 pp., and unpaginated tables.
Part 2: Crystal Descriptions, A.1 to A. 831 and Atlas of Configurations, vii pp. + unpaginated descriptions.
The two parts—£12.0.0. net ($33.60).

Published for the Barker Index Committee by W. Heffer & Sons, Ltd., Cambridge, England.

2.1.8. THE GROTH INSTITUTE

The Groth Institute discussed in the first edition of the "Directory of Continuing Numerical Data Projects", and formerly located at The Pennsylvania State University, is now associated with Nova University, Fort Lauderdale, Florida. It is still under the direction of Professor Ray Pepinsky. The Institute derives its name from Paul von Groth's "Chemische Krystallographie," a five-volume work that appeared between 1906 and 1919. The Institute was organized to collect physical, chemical, morphological, and structural data for crystals. No publications have appeared since 1960.

2.2. MINERALOGICAL PROJECTS

2.2.1. DANA'S SYSTEM OF MINERALOGY

Organization

Five editions of "The System of Mineralogy" were compiled by James Dwight Dana and published between 1837 and 1868. The author's son, Edward Salisbury Dana, compiled the sixth edition, published in 1892. The seventh edition, a complete revision and updating, was started in 1915 under the direction of Professor W. E. Ford of Yale University, but progress was slow until 1937. A number of persons in the United States and Great Britain contributed data and worked directly on the compilation. The authors of Volume I (1941) and Volume II (1944) of the seventh edition were the late Charles Palache, the late Harry Berman, and Clifford Frondel who was the sole author of Volume III (1962). Two more volumes of the seventh edition are projected. Financial aid for the first two volumes of the seventh edition was provided by the Sterling Fund of Yale University, the Penrose Funds of the Geological Society of America and the American Philosophical Society, the publishers (John Wiley & Sons, Inc.), Mr. H. S. Holden, and Harvard University. The publication is now supported entirely by Harvard University. Throughout its history, Dana's "System" has been an authoritative reference source for mineralogists.

2.2.1.

Substances

All minerals. Volume I includes elements, sulfides, sulfosalts, and oxides; Volume II contains halides, carbonates, nitrates, iodates, borates, sulfates, selenates, tellurates, selenites, tellurites, chromates, phosphates, arsenates, vanadates, antimonates, antimonites, arsenites, vanadium oxysalts, and salts of organic acids; and Volume III contains silica materials. Two more volumes are planned to cover the silicates.

Properties

Crystallographic, physical, optical, and chemical properties. The crystallographic data include interaxial angles and unit cell dimensions. Volumes I and II contain few x-ray data, but Volume III includes x-ray powder diffraction data for each substance. The physical and optical properties include color, transparency, index of refraction, hardness, melting point, cleavage, fracture, tenacity, and specific gravity. Chemical formulas, if known, and analyses are also given. The synthesis and phase relations, the type of occurrence and association in nature, and the more important localities are cited.

Sources of Data

Original articles in journals; abstracts and other secondary sources only when original papers were not available.

Critical Appraisal

All information was carefully appraised and uncertain facts were so designated. Values of interplanar spacings and of the angles, given in the tables of Volume III, were done by machine calculation. An authentic experimental diffraction pattern was obtained for each substance and optical properties were frequently checked.

Use of Nomenclature, Symbols, Units, and Physical Constants

Recommendations of international authorities such as the International Union of Crystallography and the International Mineralogical Association

are followed. There is a complete synonymy at the beginning of each species description.

Currency

The fact that the present edition is the seventh is an indication of the continuity of Dana's "System of Mineralogy" and of the esteem in which it is held. The time required to prepare the volumes of necessity prevents their being truly current. Work on Volume II was completed in the winter of 1949-1950 and some of the references are as late as 1950. In general, the cutoff date for the literature examined for Volume III was 1960, but a few more recent papers are cited. A revision of Volume I (the beginning of the eighth edition) is planned following the completion of the remaining two volumes of the seventh edition.

Format

The data are presented in text and tables in bound volumes. Volume I of the seventh edition contains an introduction and data for 8 classes of minerals; Volume II contains data for 42 classes. Volume III, devoted to silica materials, has 250 of its 334 pages devoted to quartz. References are given for each mineral description. Volume I has two bibliographic reference lists (Section 14 in the Introduction), one of which gives periodicals, the other, independent works. A general index is included in each volume.

Publication and Distribution

John Wiley & Sons, Inc., have been associated with the Dana System of Mineralogy since 1844 when they published the second edition. The current volumes are:

The System of Mineralogy of James Dwight Dana and Edward Salibury Dana, Yale University, 1837-1892, 7th edition.

Vol. I: Elements, Sulfides, Sulfosalts, Oxides; Charles Palache, Harry Berman, and Clifford Frondel, 1944, xiii + 834 pp., $14.00.

Vol. II: Halides, Nitrates, Borates, Carbonates, Sulfates, Phosphates, Arsenates, Tungstates, Molybdates, etc.; C. Palache, H. Berman, and C. Frondel, 1951, xi + 1,124 pp., $16.00.

Vol. III: Silica Minerals, C. Frondel, 1962, xii + 334 pp., $7.95.

Available from John Wiley & Sons, Inc., 605 Third Ave., New York, N.Y. 10016; and Glen House, Stag Place, London, S.W.1., England.

2.2.2. ROCK-FORMING MINERALS

Organization

"Rock-Forming Minerals" by W. A. Deer, J. Zussman, and R. A. Howie is a series of five volumes designed as a reference work for advanced students in the geological sciences but also useful to workers in other fields, particularly ceramic technologists. Though not primarily a compilation of property values, crystallographic and optical data needed for identification of rock-forming minerals are given.

Substances

Rock-forming minerals are, in the authors' words, "those which by their presence or absence, serve to determine or modify the name of a rock." The subtitles of the five volumes indicate the types of minerals included: (1) Ortho- and Ring Silicates, (2) Chain Silicates, (3) Sheet Silicates, (4) Framework Silicates, and (5) Non-Silicates.

Properties

A condensed table of properties including refractive indexes, dispersion, cleavage, twinning, color, cell dimensions, and solubilities precedes discussions that give additional property values under the heading Structure, Chemistry, Optical and Physical Properties, Distinguishing Features, and Paragenesis. Structural and phase diagrams as well as diagrams relating optical and chemical data are often given.

Sources of Data

World literature.

Critical Appraisal

The books are largely descriptive, but textual material is interspersed with property values. The chemistry sections include tables of analyses, and the relation of crystal structure to physical and chemical properties is exceptionally well presented. Data on synthetic systems, especially phase diagrams, form the basis of interpreting the composition of complex minerals. In Volume III, Sheet Silicates, the wide variability of the materials and the attendant difficulty of clear-cut definitions are well presented. This volume should be particularly interesting to ceramists. Where points of nomenclature are debatable, the authors avoid arguments by giving alternative names in parentheses. A number of reviewers have praised the books. There are few errors. Extensive references at the end of each section are an excellent guide to the literature. Abbreviations and symbols used are defined. The index lists the names and page numbers of minerals described in detail in bold type and names other than mineral names in italics.

Currency

The literature through 1959 was well covered, coverage for some sections extended through 1961, and a few references extend to 1962. It is understood that a revision is planned.

Format

The bound volumes are 6 1/4" × 10". Bold type used for mineral and authors' names in the references add to the readability of the books.

Publication and Distribution

Rock-Forming Minerals, W. A. Deer, J. Zussman, and R. A. Howie.

Vol. I: 1962, 333 pp., $16.50.
Vol. II: 1963, 379 pp., $19.50.
Vol. III: 1962, 270 pp., $16.50.
Vol. IV: 1963, 435 pp., $16.50.
Vol. V: 1962, 371 pp., $16.50.

Published by Longmans, Green and Co., Ltd., 48 Grosvenor St., London, W.1, England. Rights in U.S.A., Philippines, and Central America—John Wiley & Sons, Inc., 605 Third Ave., New York, N.Y. 10016.

2.3. OTHER SOLID STATE PROJECTS

2.3.1. ELECTRICAL AND ELECTRONIC PROPERTIES OF MATERIALS: Electronic Properties Information Center, Hughes Aircraft Company

Organization

The Electronic Properties Information Center (EPIC) was established in June 1961 at Hughes Aircraft Company, Culver City, Calif. It is administered under contract with the U.S. Air Force Materials Laboratory, Research and Technology Division, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio. Its directive is to collect, index, and abstract the literature on electrical and electronic properties of materials and to evaluate, compile, and publish the experimental data from that literature. EPIC and its publications are available to anyone wishing information within the scope of EPIC's objectives. Emil Schafer is supervisor of the center.

Substances

All materials relevant to the field of electronics. The materials covered can be divided somewhat roughly into nine categories: semiconductors, insulators, ferrites, ferroelectrics, ferromagnetics, electroluminescents, thermionic emitters, metals, and superconductors. Ceramics, originally included as a separate category, was absorbed later by the other nine. At first, data sheets were issued under a single category but, because there is considerable overlapping of the categories, later compilations have given all the pertinent properties.

Properties

Data for 29 general properties of semiconductors and for 12 properties of insulators were checked for the early compilations. Later, a consolidated list including these and about a dozen additional properties was compiled. Among the properties are cross sections, Curie constant and temperature, Debye temperature, dielectric properties, electrical conductivity and resisitivity, emission of various types, energy bands, gaps and levels, irradiation effects, and magnetic, magnetoelectric, photon, and thermal properties. Many of these are broken down into various coefficients, effects, and types so that, in all, more than 100 properties are included in searching the literature.

Sources of Data

Open literature. Abstract journals and about 40 other journals are thoroughly checked and the original articles are obtained for all personal citations. In addition, the unclassified report literature is completely searched. In some cases, values that cannot be found in the literature are calculated from available information. Evaluation of data is confined to that from primary sources unless only secondary sources are available.

Critical Appraisal

Although some of the materials for which properties are measured exist in a state of high purity—for instance, samples of semiconductors sometimes have only one part per million of impurity—other materials such as insulators may exist only in batch quantities, and values for given properties may differ markedly depending upon the raw materials and processing. Careful judgements must therefore be made as to the adequacy and comparative merit of experimental results so that the most probable values and ones that are reproducible to the extent needed by the potential users are selected. Values are selected as being the most representative, precise, and reliable, and as covering the widest range of variables. When judged doubtful, data are rejected. If equally valid property values are available from more than one source, all are given. References are given for the values recorded and sometimes for additional sources of data. The "Glossary of Electronic Properties," issued separately, defines terms and lists cross-references for properties.

2.3.1.

Use of Nomenclature, Symbols, Units, and Physical Constants

When necessary, the names, symbols, and units found in the literature are made to agree with those in general or accepted use.

Currency

Searching the literature has been both current and retrospective, the greatest attention being paid to time periods most relevant to the data sought. The procedure has been to work backward from the most recent comprehensive abstract source in a year-by-year search for a given category. The documentation activities have progressed sufficiently to enable EPIC to answer questions regarding literature and data for a number of materials for which data sheets have not yet been issued. Reappraisal of previously evaluated data is made when new values appear. At times, to fill the need for individual property values of a substance, sets of Data Sheets for those properties are issued separately but are later incorporated into a more comprehensive report.

Format

The data are published on 8 1/2" × 11" loose-leaf sheets or larger sheets folded to fit an 8 1/2" × 11" binder, stapled together as a single report or filed in a plastic comb binder. Most of the data are presented as graphs but some are in tabular form. The properties glossary is a 5" × 7" booklet.

Publication and Distribution

In addition to Data Sheets, EPIC publishes summary reviews, thesauri, glossaries, and a news bulletin. The following reports issued by EPIC, with their applicable AD-numbers and prices, may be ordered from the Clearinghouse for Federal Scientific and Technical Information, U.S. Department of Commerce, Springfield, Va. 22151.

Data Sheets

Cadmium Telluride, June 1962, 49 pp. (AD-415 331), $5.60.
Indium Phosphide, June 1962, 29 pp. (AD-414 847), $3.60.
Indium Telluride, June 1962, 27 pp. (AD-414 896), $3.60.
Magnesium Silicide, June 1962, 14 pp. (AD-414 895), $1.60.
Polyethylene Terephthalate, June 1962, 39 pp. (AD-414 846), $4.60.
Polytrifluorochloroethylene Plastics, June 1962, 20 pp. (AD-413 940), $2.60.
Zinc Telluride, June 1962, 24 pp. (AD-413 939), $2.60.
Indium Arsenide, June 1962, 57 pp. (AD-413 892), $4.60.
Aluminum Antimonide, Sept. 1962, 43 pp. (AD-413 676), $4.60.
Gallium Antimonide, Oct. 1962, 51 pp. (AD-413 775), $5.60.
Lead Telluride, Oct. 1962, 39 pp. (AD-437 311), $3.60.
Magnesium Stannide, Nov. 1962, 23 pp. (AD-413 825),$2.60.
Lead Selenide, Dec. 1962, 43 pp. (AD-437 310), $4.60.
Steatite, Feb. 1963, 49 pp. (AD-413 834), $5.60.
Beryllium Oxide, March 1963, 21 pp. (AD-413 831), $2.60.
Cadmium Sulfide, Summary Review and Data Sheets, April 1963, 155 pp. (AD-413 667), $11.50.
Magnesium Oxide, June 1963, 45 pp. (AD-413 809), $4.60.
Silicone Rubber, June 1963, 60 pp. (AD-413 906), $3.60.
Cordierite, June 1963, 25 pp. (AD-413 850), $2.60.
Forsterite, Aug. 1963, 28 pp. (AD-421 829), $3.60.
Pyroceram, Aug. 1963, 37 pp. (AD-421 883), $4.60.
Zinc Selenide, Sept. 1963, 26 pp. (AD-421 964), $2.60.
Zinc Oxide, Oct. 1963, 44 pp. (AD-425 212), $4.60.
Cadmium Selenide, Nov. 1963, 54 pp. (AD-425 216), $5.60.
Zinc Sulfide, Dec. 1963, 72 pp. (AD-427 288), $7.60.
Aluminum Oxide, March 1964, 161 pp. (AD-434 173), $4.60.
Silicon, May 1964, 209 pp. (AD-601 788), $14.50.
Borosilicate Glasses, June 1964, 115 pp. (AD-602 773), $5.00.
Sulfur Hexafluoride, Oct. 1964, 68 pp. (AD-607 949), $3.00.
Niobium, Nov. 1964, 106 pp. (AD-608 398), $4.00.
Fluorocarbon Gases, Nov. 1964, 111 pp. (AD-608 897), $4.00.
Germanium, Feb. 1965, 236 pp. (AD-610 828), $6.00.

Other Publications

EPIC Bulletin, Vol. 1, No. 1, Jan. 1965. A new monthly two-page sheet containing items of interest to users of the data sheets.

A Survey Materials Report on Tetrafluoroethylene (TFE) Plastics, J. T. Milek, Sept. 1964, EPIC Report No. S-3 (AD-607 798), $4.00.

Glossary of Electronic Properties, Emil Schafer, Jan. 1965, iv + 86 pp., EPIC Report S-7 (AD-616 783), $3.00.

Note: The following guide was compiled by the staff of EPIC but is not available from the Clearinghouse:

Electronic Properties of Materials: A Guide to the Literature, H. Thayne Johnson, ed., 2 vols., 1965, 1,700 pp., Plenum Press, New York, N.Y., $150.00. (Gives approximately 13,500 sources of experimental data on electrical and electronic properties of nearly 10,000 materials.)

2.4. INDEXES

2.4.1. INDEXES TO CRYSTALLOGRAPHIC DATA COMPILATIONS

The American Society for Testing and Materials publishes the following indexes to the Powder Diffraction File (see Section 2.1.3.). All ASTM publications are available from the American Society for Testing and Materials, 1916 Race St., Philadelphia, Pa. 19103.

a. Index to the Powder Diffraction File; Organic (Hanawalt), includes Section 1 - 16, PDIS - 15o, bound, $15.00.
b. Index to the Powder Diffraction File; Inorganic (Hanawalt), includes Section 1 - 15, PDIS - 16i, bound, $20.00.
c. Fink Inorganic Index to the Powder Diffraction File, PDIS - 16f, bound, $15.00.
d. Matthews Coordinate Index to the Powder Diffraction File, Inorganic: Termatrex Cards, $675.00; Negative-Line Cards, $185.00.

3
Nuclear Physics Projects

3.1. GENERAL NUCLEAR PROPERTIES PROJECTS

3.1.1. NUCLEAR DATA PROJECT

Organization

This project was established in 1948 at the National Bureau of Standards in Washington, D.C. In 1953 it was transferred to the National Academy of Sciences - National Research Council, Division of Physical Sciences, with financial support from the U.S. Atomic Energy Commission (AEC). In January 1964, the professional staff of seven moved to the Oak Ridge National Laboratory which is operated by the Union Carbide Nuclear Company for AEC. The project has been under the continuous direction of Katharine Way.

Substances

All nuclides.

3.1.1.

Properties

The types of data currently presented in the Nuclear Data Sheets are energy level schemes; ground state (covering data on nuclear angular momentum, nuclear magnetic-dipole and electric-quadrupole moments, abundances, and thermal neutron absorption cross sections); ground-state decay; metastable-state properties and decay; reaction data and mass-spectrometer data. Supplementary data and information provided (before 1966) include nuclear moments (Appendix 1), relative isotope abundances (Appendix 2), adjusted mass differences (Appendix 4), beta disintegration charts, energies of first 2^+-states in even-even nuclei, E2 mean-lives in even-even nuclei, a nomograph for estimating half-lives in alpha decay, beta-decay transition probabilities, and ground-state Q-values.

Sources of Data

Pertinent journals, abstracts, and reports.

Critical Appraisal

All known experimental results are reported. The compilers construct level schemes to give, in their views, the most consistent and plausible interpretations of the experimental determinations. Where choices are possible, comments on the Compilers' Analysis sheets indicate which data were selected in preparing the level schemes. The introductory material gives detailed discussions of policies, conventions, symbols, and abbreviations. A December 1964 addition to the policies section includes a 15-page discussion of spin and parity assignments with curves of gamma transition half-lives for $Z < 40$, $40 \leq Z \leq 65$, and $Z > 65$. The Compilers' Analysis sheets include reasons for all spin-parity assignments.

Use of Nomenclature, Symbols, Units, and Physical Constants

In general, the group follows the recommendations of the Commission for Symbols, Units and Nomenclature of the International Union of Pure and Applied Physics.

Currency

Additions and revisions are issued periodically.

Format

Before 1966, the 8 1/2" x 11" Nuclear Data Sheets were issued with a temporary binding from which they could be separated for filing in conventional binders. The numerical data are presented in tabular form with a literature reference for each entry. Level schemes diagrammed for an entire A-chain precede the tables. Early sheets were issued with a number indicating the year, set, and page number within the set. Beginning with the sheets issued in September 1962, the year symbol was removed and replaced by a volume number, 5 for the volume that would have been issued in 1962, to be followed by 6, 7, etc. In addition, a month and year were given to indicate the cutoff date for the data. Reference sheets follow each A-chain. Collections of Recent References were issued periodically for papers not yet covered in the data sheets. The most recent issue, containing available references to July 1964 for the region A=21 through A=212, gives a separate list for each A-chain so that the sheets can be filed with the rest of the data on that chain. From June 1961 to June 1965, pink sheets were issued with each set of data sheets. They served as news sheets for the project and gave comments or opinions from the staff and subscribers and minor corrections for sheets that had not been revised.

The data sheets are now being issued as Section B of the new journal "Nuclear Data" (see Publication and Distribution). A new system of pagination which differs slightly from that previously used is fully explained. Policies, bases for spin-parity assignments, and a cumulative index to A-chains are given in the front of the first issue of each volume. Adjusted mass differences, references, explanations of conventions, symbols, and abbreviations are given at the back of each issue. A simple method of designation on the spine of each journal indicates the A-chains covered therein. Revisions will be planned so that entire issues can be discarded.

Publication and Distribution

The 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, Nuclear Moments, and Cross Sections, September 1950, and three supplements issued April 1951, Nov. 1951, and June 1952 (out of print). Superseded by 5.
2. New Nuclear Data, Annual Cumulations, issues 24B of Vols. 6 through 10 of Nuclear Science Abstracts, Dec. 1952, 1953, 1954, 1955, and 1956. The sixth annual cumulation (1957) was issued as a separate publication by the U.S. Atomic Energy Commission. Superseded by 5.
3. Nuclear Data Cards, 1954-1957 (out of print). Superseded by 5.
4. TID-5300, Nuclear Level Schemes, A = 40 to A = 92, Sept. 1965 (out of print). Superseded by 5.
5. Nuclear Data Sheets, Jan. 1958 —. Vols. 5, and 6, 1958, 1959, 1960, 1961, published by NAS-NRC. Section B of the new journal "Nuclear Data" will be devoted to Nuclear Data Sheets. Vol. 1, No. 1, containing sheets for A-chains from A = 182 through A = 185, was issued in Feb. 1966 (see below).*
6. Radiations from Radioactive Atoms in Frequent Use, Feb. 1959, xii + 75 pp. (out of print).
7. 1959 Nuclear Data Tables, April 1959, viii + 151 pp., $1.00.†
8. 1960 Nuclear Data Tables, Parts 1 - 4, 1960.†
   Part 1: Consistent Set of Q Values, $A \leq 66$, 1961, 214 pp., $1.50.
   Part 2: Consistent Set of Q Values, $67 \leq A \leq 199$, 1961, 456 pp., $2.75.
   Part 3: Nuclear Reaction Graphs, 1960 (out of print).
   Part 4: Short Tables, 249 pp., 1961, $1.50.
9. Energy Levels of Light Nuclei, May 1962, T. Lauritsen and F. Ajzenberg, issued as Sets 5 and 6 of the 1961 Nuclear Data Sheets, essentially an addendum to a review article in Nucl. Phys., 11, 1-340 (1959). A special bound volume was issued.
10. Members of the Nuclear Data Project contributed the section Energy Levels of Nuclei, A = 21 to A = 212 of Group I, Vol. 1 of the New Series of Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology (see Section 5.1.2.).

Other publications of the Nuclear Data Project, which are not data compilations, are:

11. A Directory to Nuclear Data Tabulations, 1958, xiii + 185 pp., 70 cents.† Supplements to this directory appear in 7 and in 8, Part 4, listed above, the former covering the period Dec. 1957 to Dec. 1958 and the latter the period Dec. 1958 to June 1961.
12. Nuclear Theory Index Cards, Jan. 1958-1962 (out of print).
13. Nuclear Theory Reference Book for the following periods: 1957 and 1958, $1.00; 1959 and 1960, $1.00; and 1961 and 1962, $1.25.† All were issued in 1963 and are compilations of the corresponding Nuclear Theory Index Cards made by photographic reproduction.

14. Nuclear Theory Index Booklets, 1963—. These booklets were issued quarterly to replace the index cards 12. Current bibliographic items are presented under the same headings as used on the cards. Booklet 4 for 1963 was cumulative for the entire year. The booklets were not published for 1964, but an annual cumulation for 1964 will be published later by the U.S. Government Printing Office.

Note: The data contained in publications 1 through 4 were superseded by 5. Through Vol. 6, the sheets were issued by the Printing and Publishing Office, National Academy of Sciences - National Research Council, 2101 Constitution Ave., N.W., Washington, D.C. 20418. All correspondence relating to the content of the Nuclear Data Sheets or to availability not indicated for publications should be addressed to the Nuclear Data Group, Oak Ridge National Laboratory, P.O. Box X, Oak Ridge, Tenn. 37831.

* Subscriptions to "Nuclear Data," Section B, $15.00 per volume of 6 issues; single issues, $3.00. Reissue of most up-to-date of old sheets of A-chains (1958-1965), complete set (10 issues), $55.00; single issues, $6.50. Available from Academic Press, 111 Fifth Ave., New York, N.Y. 10003 or Berkeley Square House, London W.1, England. Section A of "Nuclear Data" will contain charged particle cross sections, reports of experimental and theoretical studies, and critical reviews. Subscriptions, $15.00 per volume of 6 issues.

† May be obtained from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, at the prices listed.

3.1.2. TABLE OF ISOTOPES*

Organization

Publication of the Table of Isotopes series began in 1940. This series was prepared in the Department of Chemistry and the Lawrence Radiation Laboratory of the University of California, Berkeley, Calif., by Glenn T. Seaborg and his associates. Since that time, extensive revisions have appeared in "Reviews of Modern Physics." The project has been supported by the U.S. Atomic Energy Commission.

Substances

All radioactive and stable isotopes of the elements.

* As a rule, compilations appearing in scientific journals would not be included in this survey. However, because of their size, viability, and continuity, exceptions have been made for this project and for projects described in Sections 3.3.1. and 3.3.2.

3.1.2.

Properties

For each isotope the following properties and related information are given when applicable and available: atomic weight, atomic number, half-life, type of decay, class, genetic relationships, percent abundance, nuclear moments (spin, magnetic, and quadrupole), energy of radiation, and disintegration energy and scheme. Supplementary tables of values such as atomic constants, energy conversion factors, and binding energies are also given.

Sources of Data

Open literature and private communications.

Critical Appraisal

Several values for half-life are often recorded with an attempt to list the most precise ones first. In some cases, where no choice is obvious, an average value is listed but is so indicated, and references for all papers whose values have contributed to the average are enumerated. Among natural radioactivities an average value taken from an international committee summary report (Rev. Mod. Phys., 3, 427, 1931) is often given. Apparent absence of a particular type of decay is indicated when no evidence for its existence has been found. The certainty of each isotopic assignment is indicated. The introduction explains in detail the plan of the compilation and the terms and abbreviations used. Complete coded references are given.

Nomenclature and Units

Recommendations of the Commission for Symbols, Units, and Nomenclature of the International Union of Pure and Applied Physics are followed, though it is not so stated.

Currency

Five tables of the series appeared between 1940 and 1958. The April 1953 table covered literature approximately through December 1952 and the April 1958 table approximately through February 1958. The tables increased in size from 17 to 320 pages. The next revision is in preparation and is expected to appear within a year.

Format

All the tables have appeared in "Reviews of Modern Physics." The tables are arranged in columns, the latest table in five columns with the following headings (1) Isotope, Z and A. (2) Half-life. (3) Type of Decay, Class, Genetic Relationships, % Abundance, Nuclear Moments. (4) Energy of Radiation in MeV. (5) Disintegration Energy and Scheme.

Publication and Distribution

Table of Isotopes, J. J. Livingood and G. T. Seaborg, Rev. Mod. Phys., 12, 30-47 (1940).

Table of Isotopes, G. T. Seaborg, Rev. Mod. Phys., 16, 1-32 (1944).

Table of Isotopes, G. T. Seaborg and I. Perlman, Rev. Mod. Phys., 20, 585-666 (1948).

Table of Isotopes, J. M. Hollander, I. Perlman, and G. T. Seaborg, Rev. Mod. Phys., 25, 469-650 (1953).

Table of Isotopes, D. Strominger, J. M. Hollander, and G. T. Seaborg, Rev. Mod. Phys., 30, No. 2, Part 2, 585-904 (1958).

The 1958 Table is obtainable from the American Institute of Physics, 335 E. 45th St., New York, N.Y. 10017.

3.1.3. TABELLEN DER ATOMKERNE (NUCLEAR TABLES)

Organization

"Nuclear Tables" is an extensive compilation of nuclear properties and reactions by Wunibald Kunz of Vienna and Josef Schintmeister,

director of the Institute for Experimental Nuclear Research at the Technische Hochschule, Dresden, Germany. The tables were compiled by the authors while they were in the Soviet Union and were later brought up to date. Part I, Nuclear Properties, was published by Akademie-Verlag, Berlin, Volume 1 in 1958 and Volume 2 in 1959. Part II, Nuclear Reactions, was published by Pergamon Press, Oxford, England, in 1965.

Substances

Part I covers the elements neutron to tin in Volume I and antimony to nobelium in Volume II. Part II covers the elements neutron to magnesium in Volume I. The elements aluminum to manganese will be covered in Volume II.

Properties

Properties for which data values are given in Part I are number of nucleons (mass number), neutrons, and excess neutrons (+ or -), atomic mass, isotopic abundance, decay, half-life, energy of particles, energy of gamma-ray quanta, conversion coefficients, and decay schemes (as diagrams). Volume I, Text Volume, of Part II gives nuclear reactions in tabular form. Cross sections are presented as numerical values and on graphs. The Q-values, threshold values, kinetic energy of emitted gamma rays, energies and quanta-characteristics of the energy levels are given in detail. A Table Volume gives detailed energy level or decay scheme diagrams.

Sources of Data

World literature as available.

Critical Appraisal

Every reference was examined in the original if it was available. In comparatively few cases, summary reports were used. After careful evaluation of the available data, the values given first in the tables were, in the judgment of the compilers, the most probable values and

in some cases were weighted mean values of those collected. Limits of error are generally given. Values within the limits of error of those in first place are not repeated, but references for them are given in chronological order. Complete references are given. Values calculated by the authors from available data are indicated by the letters "SK." The preface and explanation of the tables of both parts are given in English, German, and Russian. Symbols and abbreviations used are defined, and sample entries of data and decay schemes are discussed in detail.

Currency

Part I includes all data available to the authors published between January 1, 1940, and January 1, 1958. Part II, Volume 1, includes many references to articles published from 1958 to 1962. Part II, Volume 2, is scheduled for publication in late 1966.

Format

Part I, Volumes 1 and 2, and Part II, Volume 1, Text Volume, are clothbound books, 8 1/2" x 11 3/4". The Table Volume of Part II, Volume 1, consists of 36 energy level diagrams, some requiring two or three sheets that vary in size from 16 1/2" x 11 1/2" to 33" x 23". The sheets are folded to 8 1/4" x 11 1/2" and contained in a cardboard box cover 9" x 12 1/4".

Publication and Distribution

Tabellen der Atomkerne (Nuclear Tables), W. Kunz and J. Schintlmeister. Teil (Part) I, Eigenschaften der Atomkerne (Nuclear Properties); Band (Volume) 1, Die Elemente Neutron bis Zinn (The Elements Neutron to Tin), 1958, xliv + 465 pp. Akademie-Verlag, G.m.b.H., Berlin W.8, Mohrenstrasse 39, Germany, price, 105 DM ($26.25). Teil I, Band 2, Eigenschaften der Atomkerne, Die Elemente Antimon bis Nobelium (Antimony to Nobelium), 1959, xliv + 641 pp. (466-1,107), price, 130 DM ($32.50). Akademie-Verlag, Berlin. (Also available from Pergamon Press,* £20.0.0. per set.)

Part II, Nuclear Reactions, Vol. 1, The Elements from Neutron to Magnesium, Text Volume, xliv + 700 pp. Table Volume, 36 tables (five of which require 2 or 3 sheets), 1965. Price £25.0.0. ($75.00) for the two volumes.

*Pergamon Press, Headington Hill Hall, Oxford, England; 4/5 Fitzroy Square, London, W.1, England; 122 E. 55th St., New York, N.Y. 10022.

3.2. CROSS-SECTION PROJECTS

3.2.1. NEUTRON CROSS SECTIONS, Brookhaven

Organization

The Sigma Center of Brookhaven National Laboratory, Upton, N.Y., is the site of this program. Sponsored and financed by the U.S. Atomic Energy Commission, the program was coordinated by Donald J. Hughes until his death in April 1960. Beginning in 1961, it was under the direction of John R. Stehn and is now under the direction of Murrey D. Goldberg with a staff of four scientists and three clerical workers.

Substances

All nuclides and natural occurring mixtures of isotopes.

Properties

Neutron cross-section data are presented as thermal cross sections, resonance parameters, cross-section curves, and angular distributions. Thermal cross sections include reaction cross sections (absorption and activation) and scattering cross sections (coherent, incoherent, bound atom, and average) for thermal or 2,200 m/s neutrons. Resonance parameters are given for light, heavy, and fissionable nuclei. The cross-section curves cover several energy ranges, from zero to more than 10^8 eV. The majority of the angular distribution curves are for elastically scattered neutrons but a large number are for inelastically scattered neutrons; some are for charged particles and for gamma rays associated with inelastic neutron scattering. Not included are angular distributions of fission fragments or of fission neutrons, distributions for which the neutron source is a fission spectrum, and distributions for the inelastic scattering of slow neutrons.

Sources of Data

Open literature and unpublished work available to the authors.

Critical Appraisal

The publications of this project are intended to serve primarily the needs of reactor physicists and engineers, but an attempt has been made to present the data in the form most useful to physicists in general as well as to reactor specialists. In the most recent issues, emphasis has been placed on nuclear processes involved rather than on methods of observation. Except for the recommended values and the curves, all recorded values are experimental. The recommended values for which estimated errors are given are, in general, weighted means of the experimental values. The compilers drew the smoothed curves through the points on the graphs with no attempt to perform a least-squares fit to any predetermined shape. They emphasize that a curve represents their own idea of a reasonable fit to the data and not the opinion of the original authors.

Currency

Supplements are issued and revisions made at irregular intervals. Unpublished contributions from individuals result in the presentation of many very recent values. The second edition of "Angular Distributions" (BNL 400), includes data available in October 1962. Volume I (Z = 1 to 20) of the second supplement to the second edition of "Neutron Cross Sections" (BNL 325), was issued in August 1964. The information closing date was May 1964. Volume II (Z = 21 to 87) is being issued in several volumes. Volume IIA (Z = 21 to 40), with a closing date of February 1966, was issued in July 1966; Volume III (Z = 88 to 98), with a closing date of February 1965, was issued in July 1965. Volume IIB (Z = 41 to 60) is in press. The manuscript for Volume IIC (Z = 61 to 87) is completed. Publication is expected during the winter of 1966-1967.

Format

The second edition and first supplement of "Neutron Cross Sections" (BNL 325) are 10 1/4" x 15 1/2" paperback books. The second supplement is issued as 8 1/2" x 11" loose-leaf sheets with heavy paper covers in plastic-comb binders. The graphs are greatly reduced in size and more of them have linear coordinates instead of the log-log or semilog coordinates that were predominant in the

earlier issues. "Neutron Cross Sections—Angular Distributions" (BNL 400) is issued as 8 1/4" x 10 3/4" paperback books, the two-volume second edition bound with plastic-comb paper binders as above.

The angular distribution data are plotted on linear grids. Textual references, laboratory in which the measurements were made, type of experiment, and other pertinent information are given on a left-hand page facing the graphs. The earlier issues of both BNL 325 and BNL 400 were paginated consecutively; those since 1962 use a three-number system that denotes the atomic number, the isotope, and the page for a given element and isotope. The elements are arranged in order of their increasing atomic numbers.

Publication and Distribution

AECU 2040, May 1952, superseded by BNL 325.
BNL 325, Neutron Cross Sections, July 1955, v + 328 pp. (includes angular distributions).
BNL 325, Supplement 1, January 1957, xxvii + 129 pp.
BNL 325, 2nd edition, July 1958, v + 373 pp. Supersedes 1st edition and its supplement 1, $4.50.*
BNL 325, 2nd edition, Supplement 1, January 1960, iv + 129 pp., $2.00.*
BNL 325, 2nd edition, Supplement 2, Vol. I, Z = 1 to 20, May 1964, sectional pagination, $2.50.*
BNL 325, 2nd edition, Supplement 2, Vol. IIA, Z = 21 to 40, February 1966, sectional pagination, $4.00.†
BNL 325, 2nd edition, Supplement 2, Vol. IIB, Z = 41 to 60; in press.
BNL 325, 2nd edition, Supplement 2, Vol. IIC, Z = 61 to 87; in preparation.
BNL 325, 2nd edition, Supplement 2, Vol. III, Z = 88 to 98, February 1965, sectional pagination, $3.00.†
BNL 400, Neutron Cross Sections—Angular Distributions, June 1956, 102 pp.†
BNL 400, 2nd edition, Angular Distributions in Neutron-Induced Reactions, Vol. I, Z = 1 to 22, Vol. II, Z = 23 to 94, October 1962, 804 pp., sectional pagination, $8.50.†

* Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

† Available from the Clearinghouse for Scientific and Technical Information, Springfield, Va. 22151.

3.2.2. NEUTRON CROSS SECTIONS, Livermore

Organization

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

Substances

All nuclides and natural occurring elements.

Properties

Experimental values of total and reaction neutron cross sections in the energy range from 0.001 to 14.5 MeV (Part I); semi-empirical cross-section curves for the energy range 0.5 to 15.0 MeV and a table of threshold energies for neutron reactions (Part II); and differential neutron cross sections for the energy range 0 to 15 MeV (Part III). Thresholds of nuclear reactions for the various impinging particles were issued as a new compilation in 1964.

Sources of Data

Journals, AEC report literature, and private communications.

Critical Appraisal

In the first edition of "Tabulated Neutron Cross Sections" (May 1958), no selection of values was made; essentially all available experimental data were presented. In the completely revised second edition (October 1959), an effort was made to eliminate clearly superseded data, but in a few cases more than one set of data is given. In Part II, calculations were used to supplement data where there was a shortage of measured values or where ambiguity existed between several values. In Part III, an effort was made to select the best values available. Limits of measurement are indicated in Parts I and III.

3.2.2.

Use of Nomenclature, Symbols, Units, and Physical Constants

Symbolism in this field is not well established. The notation system used is completely defined in order to avoid ambiguity.

Currency

Originally data were presented on loose-leaf sheets so that issuance of new sheets could keep the compilations relatively current. The only replacement sheets issued have been those in the complete revision of Part I in October 1959. This is because a tape library of experimental and evaluated neutron cross sections was set up in 1960 and is maintained on a more or less updated basis.

Format

Loose-leaf sheets 8 1/2" x 11" are contained in specially printed plastic-covered binders. Part I, "Tabulated Neutron Cross Sections," is completely tabular and consists of three volumes. Sources of data are identified in the tables by numbers referring to a complete reference table included in each volume. Part II, "Semi-Empirical Neutron Cross Sections," contains cross-section energy curves preceded by a 146-page textual section that includes a general discussion of the cross-section systematics and a detailed discussion of the curves of each element or isotope. Most graphs contain several curves such as total, nonelastic, elastic scattering, inelastic scattering, and specific reaction neutron cross sections plotted against energy. No references to original data sources are given because the data of Part I are used, but an annotated bibliography is given for supplemental information. Part III, "Tabulated Differential Neutron Cross Sections," presents data in tabular form. The references are the same as those in Part I with the addition of 17 more recent ones (total, 584). No indexes are provided, because the material in each volume is arranged in order of increasing atomic numbers of the elements and, in turn, the mass numbers of the isotopes. The values in the threshold charts are also arranged in order of Z numbers with a separate section for each impinging particle, that is, neutron, proton, deuteron, triton, He^3, $He^4(\alpha)$, and γ (photon).

Publication and Distribution

Part I, Tabulated Neutron Cross Sections, 0.001 - 14.5 MeV., R. J. Howerton, Vol. I, $_{1}H$ - $_{22}Ti$; Vol. II, $_{23}V$ - $_{50}Sn$; Vol. III, $_{51}Sb$ - $_{95}Am$; UCRL-5226, first edition, May 1958. UCRL-5226, revised, 1959; Vol. I, $5.00, Vol. II, $5.00, Vol. III, $4.00.

Part II, Semi-Empirical Neutron Cross Sections, 0.5 - 15 MeV., $_{1}H$ - $_{94}Pu$, R. J. Howerton, Vol. I, Nov. 1958, UCRL-5351. (Photostat copy, $37.80, Microfilm copy, $11.10, available from the Library of Congress.)

Part III, Tabulated Differential Neutron Cross Sections, $_{1}H$ - $_{94}Pu$, R. J. Howerton, Vol. I, Jan. 1961, UCRL-5573, $5.00.

Parts I and III may be obtained from the Clearinghouse for Scientific and Technical Information, Springfield, Va. 22151.

Thresholds of Nuclear Reactions, R. J. Howerton, Donald Braff, W. J. Cahill, and Nanette Chazan.

Neutron Induced Reactions, UCRL-14,000, May 1964.
Proton Induced Reactions, UCRL-14,001, Sept. 1964.
Deuteron Induced Reactions, UCRL-14,002, Sept. 1964.
Triton Induced Reactions, UCRL-14,003, Sept. 1964.
He^3 Induced Reactions, UCRL-14,004, Sept. 1964.
He^4 Induced Reactions, UCRL-14,005, July 1964.
Photon Induced Reactions, UCRL-14,006, Sept. 1964.
Tabulated Neutron-Induced Gamma Production Cross Sections for Primary Neutron Energies of 0.1 to 14 MeV, Nanette J. Chazan, UCRL-14,007, Revision 1, Aug. 1965.

A limited number of the 14,000 series are available from the director of the project upon request. UCRL-14,007 may be obtained from the Clearinghouse, $4.00 for "hard copy" and 75 cents for microfiche copies.

3.2.3. CHARGED-PARTICLE CROSS SECTIONS, Oak Ridge National Laboratory

Organization

This project, sponsored by the U.S. Atomic Energy Commission (AEC), is carried on in the Charged-Particle Cross-Section Data Center of the Physics Division at Oak Ridge National Laboratory

(ORNL) under the supervision of Francis K. McGowan. The program originated at Los Alamos Scientific Laboratory about 1955. It was discontinued in 1960, and after a brief lapse was started again at ORNL.

Substances

In scope, the compilation includes cross-section data at all energies for nuclear reactions of the type A(x,y)B, where A is the target nucleus and B the residual nucleus, x is the bombarding charged particle, and y is the outgoing particle or particles in the reaction. The mass of x must be equal to or greater than one nucleon mass. To date, only targets from hydrogen (as proton, deuteron, and triton) through copper have been covered. Bombarding particles have included p, d, t, α, ^{3}He, ^{6}Li, ^{12}C, ^{14}N, ^{16}O and in a few isolated reactions ^{15}N, ^{19}F, ^{20}Ne, and ^{22}Ne.

Properties

Cross-section data at all energies including angular distributions and excitation functions; angular dependence of polarization produced in elastic scattering. Nuclear reactions involving mesons in the exit channel are not included.

Sources of Data

Open literature, AEC reports, and preprints of papers to be published. Nuclear Science Abstracts, Physics Abstracts, and Chemical Abstracts are used as sources to maintain a bibliography.

Critical Appraisal

In general, only one reference is given for each set of data. This was either the only set available or the best set in the opinion of the compiler. Errors of the cross sections given in the caption are standard deviations. When the type of error is not designated by the author, the compiler has arbitrarily assumed that the errors were standard deviations. In many early cross-section data the only source

was a small figure in a journal. A Moseley model 2S X-Y point plotter was used to read the points from these small figures. The components of the reader provide an over-all accuracy of ± 0.25 percent of full scale. In general, the accuracy of the data points read from the small figures depends on the accuracy of graphic arts in the original drawing and on the distortions produced by the publisher; such accuracy would not be increased by enlargement of the figures. The caption to the tabular data includes the reaction, often the energy E (in the laboratory frame of reference) and the energy of the merging particle (or particles) Q (taken from the 1961 Nuclear Data Tables), the reference, contributing laboratory, a few experimental details, and source of tabular data. In most cases, some expression of the errors is given in either the caption or the tabulated data.

Use of Nomenclature, Symbols, Units, and Physical Constants

In general, the symbols used conform to those in use by the Nuclear Data Project (Section 3.1.1.) and recommended by the Commission for Symbols, Units and Nomenclature of the International Union of Pure and Applied Physics (see Appendix). The symbols for several quantities were different in the ORNL compilation from those used in the Los Alamos compilations—for example, angle in center-of-mass system: Los Alamos, θ', ORNL, θ; angle in laboratory frame of reference: Los Alamos, θ, ORNL, Ψ. However, lists of symbols and abbreviations are given in LA-2014 and ORNL-CPX-1.

Currency

The first report issued by the Los Alamos group appeared in February 1957 and covers literature through January 1956. The second, dated January 1961, covers literature before January 1, 1960. The two reports cover targets hydrogen through fluorine, and neon through chromium, respectively. The first compilation by the ORNL group, issued in July 1964, covers manganese, iron, and cobalt, the second, issued in January 1965, covers nickel and copper. Both include the literature before January 1, 1964. The plan is to finish the first cycle of the compilation, that is, the group from nickel through uranium, in probably three or four sections, and concurrently to bring the cross-section data up to date for the light elements. Future issues of data will appear in Section A of the new journal "Nuclear Data" (see Publication and Distribution Section).

3.2.3.

Format

Both compilations from Los Alamos, LA-2014 and LA-2424, consist of graphs only, with smooth curves drawn. LA-2014 is composed of loose-leaf sheets, 11" x 17"; LA-2424 is paperbound with 9 1/4" x 14" sheets. The ORNL compilations are white plastic-covered many-slot loose-leaf binders for 8 1/2" x 11" sheets. Data are presented in tabular and graphic form on facing pages. All cross-section data, including both angular distributions and excitation functions, are presented on semilog graph paper, and the angular dependence of the polarization produced in the elastic scattering reaction is presented on linear graph paper. No curves are drawn, and data points are plotted. A number of bibliographies for data not plotted, energy spectra, relative data, and angular correlation data are given in appendixes.

Publication and Distribution

LA-2014, Charged Particle Cross Sections, Nelson Jarmie and John D. Seagrave, eds., Feb. 1957, 234 pp., $1.25.

LA-2424, Charged Particle Cross Sections, Neon to Chromium, Darryl B. Smith, Compiler and ed., Nelson Jarmie and John D. Seagrave, associate eds., Jan. 1961, iii + 137 pp., $2.50.

LA reports available from the Clearinghouse for Scientific and Technical Information, Springfield, Va. 22151.

ORNL-CPX-1, Nuclear Cross Sections for Charged-Particle Induced Reactions, Mn, Fe, Co, F. K. McGowan, W. T. Milner, and H. J. Kim, compilers, July 1964, 443 pp.

ORNL-CPX-2, Nuclear Cross Sections for Charged-Particle Induced Reactions, Ni, Cu, F. K. McGowan, W. T. Milner, and H. J. Kim, compilers, Sept. 1964, iii + 511 pp.

ORNL reports available on request from Charged-Particle Cross Section Data Center, Oak Ridge National Laboratory, P.O. Box X, Oak Ridge, Tenn. 37831.

New sections of Charged-Particle Cross Sections as they appear will be published in Section A of "Nuclear Data, A Journal Devoted to Compilations and Evaluations of Experimental and Theoretical Results in Nuclear Physics." Volume 1, 1965-1966, will consist of six issues. No. 1 appeared in December 1965, No. 2 in February 1966. Subscription price, $15.00 per volume.

Published by Academic Press, 111 Fifth Ave., New York, N.Y. 10003; or Berkeley Square House, London, W.1, England.

3.3. ENERGY LEVEL PROJECTS

3.3.1. ENERGY LEVELS OF LIGHT NUCLEI, ^{5}He to ^{24}Ne*

Organization

Six reports under the above title have been published since 1948. Being reviews as well as compilations, they summarize experimental information on the energy level schemes of the nuclei from ^{5}He to ^{24}Ne. Professor Thomas Lauritsen of the California Institute of Technology has been an author (Report II) or coauthor of all the reports. Professor Fay Ajzenberg-Selove of Haverford College has coauthored Reports III to VI. The work has been supported in part by the U.S. Air Force through the Office of Scientific Research, by the joint program of the U.S. Office of Naval Research and the U.S. Atomic Energy Commission, and by the National Science Foundation. This project complements rather then duplicates the project discussed in Section 3.3.2.

Substances

Light nuclei, ^{5}He to ^{24}Ne (Z = 2 to Z = 10).

Properties

Energy level schemes and the nuclear reactions in which they are involved are presented. Excitation energies, masses, Q-values, binding energies (weighted mean values), resonances, γ-transitions, and cross sections are among the properties reported. A separate table of atomic mass excesses is included.

* See footnote to Section 3.1.2.

Sources of Data

Open literature and prepublished data.

Critical Appraisal

The data upon which the level schemes are based are tabulated, analyzed, and discussed for each nuclide covered. Coded references are given.

Currency

References cited indicate that the literature very close to the date of the manuscript was reviewed.

Publication and Distribution

Energy Levels of Light Nuclei

I: W. F. Hornyak and T. Lauritsen, Rev. Mod. Phys., 20, 191-227 (1948).
II: T. Lauritsen, Nat. Acad. Sci. - Nat. Res. Council, Nucl. Sci. Rept., 5, 52 pp. (1949); out of print.
III: W. F. Hornyak, Thomas Lauritsen, P. Morrison, and H. A. Fowler, Rev. Mod. Phys., 22, 291-372, (1950).
IV: F. Ajzenberg and T. Lauritsen, Rev. Mod. Phys., 24, 321-402 (1952).
V: F. Ajzenberg and T. Lauritsen, Rev. Mod. Phys., 27, 77-166 (1955).
VI: F. Ajzenberg-Selove and T. Lauritsen, Nucl. Phys., 11, 1-340 (1959). This report may be obtained for $10.00 from North Holland Publishing Company, P.O. Box 103, Amsterdam, the Netherlands.
VII: In preparation.

3.3.2. ENERGY LEVELS OF LIGHT NUCLEI, Z = 11 to Z = 20*

Organization

A series of three compilations under the above title have been published since 1954, compiled by P. M. Endt and his colleagues of the Fysisch Laboratorium der Rijksuniversiteit, Utrecht, the Netherlands. This series, reviews as well as compilations, complements rather than duplicates the project discussed in Section 3.3.1.

* See footnote to Section 3.1.2.

Substances

Light nuclei, Z = 11 to Z = 20.

Properties

Energy levels are given in both tabular and schematic form. Weighted mean values of excitation and resonance energies are given. Tables of atomic mass excesses, natural abundance, and nuclear moments are also given.

Sources of Data

Open literature and private communications.

Critical Appraisal

Errors in energies (reported in MeV) are at most 5 units in the last decimal. Doubtful levels or transitions are marked by hatched lines, and uncertain values are bracketed. Analytical discussions of the selection of data are given for each nuclide.

Currency

The articles have appeared at three- or four-year intervals. Each one is complete in itself in that it brings the data up to date. However, papers of only historical interest or those that have been superseded have been omitted from the later bibliographies. Article III, for which the manuscript was submitted in November 1961, contained references up to October 1, 1961, but references (with short discussions and data) for articles received from October 1, 1961, to February 15, 1962, were included as addenda immediately following Article III in Nuclear Physics. The data of the addenda are not incorporated in the figures and master tables of the main text.

Publication and Distribution

Energy Levels of Light Nuclei, Z = 11 to Z = 20

I: P. M. Endt and J. C. Kluyver, Rev. Mod. Phys., 26, 95-166, (1954).

II: P. M. Endt and C. M. Braams, Rev. Mod. Phys., 29, 683-756 (1957).

III: P. M. Endt and C. van der Leun, Nucl. Phys., 34, 1-324 (1962). Reprints of this paper are obtainable for $10.00 from North Holland Publishing Company, P.O. Box 103, Amsterdam, the Netherlands.

IV: In preparation.

3.3.3. DECAY SCHEMES OF RADIOACTIVE NUCLEI

Organization

Two editions with the above title have appeared since 1958. They were published in Russian by the U.S.S.R. Academy of Sciences Press. The first was by B. S. Dzhelepov and L. K. Peker, the second by the same authors with V. O. Sergejev as a coauthor. The first edition has been translated into English and published by Pergamon Press.

Substances

The first edition treated radioactive nuclei from A = 1 to A = 256, the second edition, nuclei from A = 100 to A = 257.

Properties

Decay scheme diagrams of radioactive nuclei, i.e., the ground and excited states of nuclei and the probabilities of different transitions between them. The second edition, in addition to the data on levels excited in radioactive decay, includes data on levels excited in different nuclear reactions, such as Coulomb excitation (n,r), (d,p). Numerical values referring to energy levels and transitions between them are placed directly on the diagrams. Scale changes are indicated by breaks in the lines. Mass, isotopic abundance, half-life, transition energies, and other information are given on the diagrams. Tables at the end of the second edition give spin values, magnetic dipole and electric quadrupole moments, conventional names of radioactive isotopes, binding energies of electrons, cross sections of nuclear

activation by thermal neutrons, and nomograms for calculation of log ft, for β^--, β^+-, and ϵ-transitions.

Sources of Data

World literature.

Critical Appraisal

Both editions give the title page and introduction in English and Russian and give the English meanings of abbreviations. The introduction has an excellent description of the decay scheme diagrams and supplementary data. The second edition has a two-page list defining symbols in Russian only, probably because the symbols throughout the book are in roman characters. The decay scheme diagrams are explained in Russian with the use of a typical scheme. On a diagram, all the isotopes with the mass number A are given at the top of the page by chemical symbol, with mass number as a right superscript, atomic number as a left superscript, and number of neutrons in the nucleus as a right subscript, in part contrary to the International Union of Pure and Applied Physics recommendations. Supplementary information and a bibliography are given for each nuclide.

Currency

The decay scheme diagrams of the first edition, published in 1958, were constructed from experimental data published up to the end of 1957. The diagrams of the second edition (1963) were based on data published and available to the authors up to April 1962. Many of the schemes of the first edition were revised for the second edition.

Format

The first edition of the Russian text is a well-bound 7" x 10 1/2" book printed on good-quality paper. The second edition is the same size, but has a less attractive binding and paper of much poorer quality. The printing is clear in both text and diagrams. The English translation is a well-bound book 6 3/4" x 10". Addenda of new references are given at the end of each addition.

3.3.3.

Publication and Distribution

Decay Schemes of Radioactive Nuclei, B. S. Dzhelepov and L. K. Peker, 1958, viii + 787 pp., USSR Academy of Sciences Press, Moscow and Leningrad.
English translation of above, 1961, vi + 786 pp., Pergamon Press, New York, Oxford, London, Paris.

Decay Schemes of Radioactive Nuclei, $A \geq 100$, B. S. Dzhelepov, L. K. Peker, and V. O. Sergejev, 1963, 1,060 pp., USSR Academy of Sciences Press, Moscow and Leningrad.

4 Spectral and Other Atomic and Molecular Projects

4.1. ATOMIC SPECTRA

4.1.1. ATOMIC ENERGY LEVELS (AND AN ULTRAVIOLET MULTIPLET TABLE)

Organization

This project was established at the National Bureau of Standards (NBS) in 1946 with the encouragement of the National Academy of Sciences - National Research Council Committee on Line Spectra of the Elements. The project is under the supervision of Charlotte E. Moore-Sitterly of the Spectroscopy Section of the Atomic Physics Division, Institute for Basic Standards.

Substances

As far as possible, all the elements are to be covered.

4.1.1.

Properties

Only those energy levels are presented that are derived from observations of atomic spectra exclusive of hyperfine structure ascribed to atomic nuclei (except for hydrogen, deuterium, and tritium).

Besides relative values of derived energy levels, information is given on term designations, intervals, quantum numbers, magnetic splitting factors, electron configurations, and ionization potentials. As the tables on atomic energy levels do not include the lists of observed spectral lines from which the atomic energy levels are derived, a table titled "An Ultraviolet Multiplet Table" covering the same range of elements is issued to accompany each volume of "Atomic Energy Levels." The data given for each wavelength include intensity, excitation potentials, J-values and multiplet designations, and multiplet numbers.

Sources of Data

The open literature, unpublished results, and a comprehensive card catalog of data and references, kept up to date since 1914 at NBS, constitute the main sources of data. Collaborators outside NBS, both in the United States and abroad, supply unpublished material on spectrum analysis.

Critical Appraisal

The data are carefully examined and appraised by the staff or outside collaborators recognized as authorities in their field. The demand for reprintings of both "Atomic Energy Levels" and "An Ultraviolet Multiplet Table" is a measure of the esteem in which these compilations are held.

Use of Nomenclature, Symbols, Units, and Physical Constants

The terminology and constants used are those generally accepted by spectroscopists and are adequately explained or defined in the introductory material. A special effort has been made to introduce a uniform scheme of spectroscopic notation. In the second edition (see next section) the new revised conversion factor from reciprocal centi-

meter to electron volt has been used to obtain the respective ionization and excitation potentials quoted in the tables.

Currency

The elements are treated systematically in order of their atomic numbers. Volume I appeared in 1949, Volume II in 1952, and Volume III in 1958; Volume IV is still in preparation. Volume II contains a list of additions and corrections to Volume I, and Volume III contains a similar list for both Volume I and Volume II. Volume IV will include the lanthanide and actinide groups of elements. The complexity of the remaining spectra and the large amount of new data to be determined make the preparation of Volume IV a formidable undertaking that may well take 8 to 10 years for completion. The card catalog of data and references is kept current at all times.

Section 1 of a second edition of both the Atomic Energy Levels and the Multiplet Tables was issued in June 1965 as a publication in the National Standard Reference Data Series. The plan is to include revised "Atomic Energy Levels" and "Selected Multiplets" as Parts A and B of the same volume and to publish a section of the tables whenever the analysis of a spectrum has reached the stage where no further revision or extension is likely to occur in the foreseeable future.

Format

"Atomic Energy Levels" is published as a 9 1/8" x 11 1/4" page book. The tabular form of presentation resulted from a census of the opinions of interested workers in the various fields of science. The spectra are indexed and arranged in order of the increasing atomic numbers of the elements. References, given for each spectrum, cover the complete analysis and are labeled according to content: classified lines, energy or Grotrian diagrams, Zeeman data, and the like. "An Ultraviolet Multiplet Table" is a paperback booklet, also with 9 1/8" x 11 1/4" pages. Data are presented in seven-column tables, the elements being treated in order of increasing atomic number. References precede each table.

The paging system of the new revision will permit the arrangement of the various sections by atomic numbers regardless of the order in which the sections are published. The page size and form of the tables are the same as in the first edition.

4.1.1.

Publication and Distribution

Atomic Energy Levels As Derived from the Analyses of Optical Spectra, Charlotte E. Moore, NBS Circular 467.

Vol. I: Hydrogen to Vanadium (Z = 1-23), 1949, 309 pp., $5.50.
Vol. II: Chromium to Niobium (Z = 24-41), 1952, 227 pp., $4.00.
Vol. III: Molybdenum to Lanthanum (Z = 42-57) and Hafnium to Actinium (Z = 72-89), 1958, 245 pp., $3.00.
Vol. IV: Lanthanide and Actinide groups; in preparation.

(Demand for these volumes has been so great that Volume I was reprinted in 1950, 1954, 1960, and 1964; Vol. II in 1958 and 1963; and Vol. III in 1963.)

An Ultraviolet Multiplet Table, Charlotte E. Moore, NBS Circular 488.

Section 1, 1950, 85 pp., reprinted 1956.
Section 2, 1952, 120 pp., reprinted 1956.
Combined Sections 1 and 2, reprinted 1963, $1.25;
Section 3, 1962, 98 pp., 60 cents.
The first three sections include spectra of the elements in the corresponding volumes of Circular 467.
Section 4, 1962, 70 pp., 45 cents.
A Finding List for spectra of elements in Sections 1 and 2.
Section 5, 1962, 34 pp., 30 cents.
A Finding List for spectra of elements in Section 3.

Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables Si ii, Si iii, Si iv, NSRDS-NBS 3, Section 1, Charlotte E. Moore, June 1965, 40 pp., 35 cents.

The above reports are available, at the prices given, from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

Note: Although not part of this project, another publication by Charlotte Moore of great current importance was reprinted by NBS. This is "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, 1959 (PB 151395), and is obtainable for $4.00 from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Va. 22151.

4.1.2. ATOMIC TRANSITION PROBABILITIES

Organization

Needs in the fields of plasma physics, astrophysics, and space research have led to rapid growth in the field of atomic spectroscopy within the last six years. In 1960, a Data Center of Atomic Transition Probabilities was established at the National Bureau of Standards (NBS) to survey the available literature and to produce critical compilations of data in this field. The Center is under the direction of W. L. Wiese. The project is supported by the Department of Defense Advanced Research Project Agency. The first data compilation of the Center was issued as one of the new NBS National Standard Reference Data Series.

Substances

The first and second volumes (the latter in preparation) cover the first 20 elements of the Periodic Table. Succeeding volumes will probably not follow this systematic order but will include elements for which extensive and worthwhile data are available, primarily the heavier noble gases, some of the well-known metals, the alkalies, the alkaline earths, and eventually the remaining elements.

Properties

Ground state, ionization potential, and for both allowed transitions and forbidden transitions (when given) the following: spectroscopic notation, wavelength, energy levels, statistical weights (g_i and g_k), transition probability for spontaneous emission (A_{ki}), and line strength (S). In addition, for allowed transitions, absorption oscillator strength and log gf; and for forbidden transitions, type of transition.

Sources of Data

Compilations of Charlotte Moore-Sitterly (see Section 4.1.1.), world literature, and private communications. Calculations based mainly on the Coulomb approximation of Bates and Damgaard have been made

to fill gaps for which experimental and other theoretical values were not available.

Critical Appraisal

The introduction includes discussions of the major experimental and theoretical methods by which the tabulated data were obtained. In addition, a brief introduction for each ion points out the major reasons for selection of the tabulated values and gives some indication of their accuracy. The goal was to list all the stronger lines characteristic of the ions and additional material with uncertainties less than 50 percent. The estimation of uncertainties is coded to indicate those within 1, 3, 10, 25, and 50 percent and those larger than 50 percent. According to the authors, the only transition probabilities known with an accuracy comparable to that of wavelengths are those for hydrogen and hydrogen-like ions and for a few transitions of helium. The values recorded contain as many digits as are consistent with the estimated accuracy of the data. When values were obtained by several methods of comparable quality, the results were averaged to obtain the "best value." Abbreviations and symbols used are explained in a short appendix.

Currency

Most of the literature through 1963 was examined. A few 1963 references, found too late for their data to be included, are listed. The plan is to extend the compilation to other elements and to issue revisions when necessary.

Format

Publication is in a cloth-bound volume, 9 1/4" x 11 5/8".

Publication and Distribution

Atomic Transition Probabilities, A Critical Data Compilation; Vol. I, Hydrogen Through Neon, W. L. Wiese, M. W. Smith, and B. M. Glennon (NSRDS-NBS 4, Vol. I), May 1966, xi + 154 pp., $2.50.

Other related publications, not compilations of data:
Two editions of Bibliography on Atomic Transition Probabilities, B. M. Glennon and W. L. Wiese: (1) NBS Monograph 50, 1962, 44 pp., superseded by (2) NBS Miscellaneous Publication 278, 1966, 92 pp., 55 cents.

The above publications are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

4.2. INFRARED AND MICROWAVE SPECTRA

4.2.1. SELECTED INFRARED SPECTRAL DATA (Category B): American Petroleum Institute Research Project 44

Organization

The American Petroleum Institute (API) Research Project 44, described in Section 1.1.2., initiated a catalog of infrared spectral data in 1943, the first compilation of its kind in the field. The project accepts infrared spectra for the compilation from selected industrial, academic, and governmental laboratories. Bruno J. Zwolinski, director, Thermodynamics Research Center at Texas A&M University, College Station, Texas, is in charge of the spectral data program.

Substances

Principally hydrocarbons, but also oxygen, nitrogen, and sulfur derivatives of the hydrocarbons and a few metallic hydrides and organometallic compounds.

Properties

Infrared absorption spectra mostly in the range 2 - 15 μ but some in ranges 14 - 25 μ and 14 - 40 μ. Percent transmittance is in most cases plotted against both wavelength in microns and frequency in reciprocal centimeters. For some spectra, only one unit is indicated. Numerical values of principal peaks and shoulders are tabulated for

some spectra. Data in the far infrared are now being collected by the supporting experimental program of the Chemical Thermodynamic Properties Center. (Other compilations of API Research Project 44 are discussed in Sections 1.1.2., 4.3.1., 4.4.1., 4.5.1., and 4.6.1.)

Sources of Data

Spectra measured in 51 qualified cooperating laboratories in the United States and in a few laboratories in Canada, England, and Japan are included in the catalog as of June 30, 1966.

Critical Appraisal

Spectra are selected from those submitted by contributing laboratories, on the basis of the competence of the investigator, the quality of the instrumentation employed, and the purity of the compounds. Currently, emphasis is placed on grating spectra of high resolution. Inferior spectra are replaced as better ones become available. The source and purity of the compound is given in the legend when possible. To upgrade quality, the project supplies contributors with instructions for use of selected commercial instruments, giving techniques for calibration for absolute wavelengths and intensities.

Currency

Revisions and additions are issued semiannually when warranted by the accumulation of new spectra.

Format

The spectra are published on 8 1/2" × 11" loose-leaf sheets, for which special post binders are available. The sheets are arranged by serial number. Most of the spectrograms consist of two strips extending from 2 to 9.5 μ and from 9 to 15 μ. The name of the contributing laboratory is given on the spectral sheet and identified in the indexes by code letters. A compound index, based on the Standard Order System and in turn on compound type, and a numerical index arranged in order of serial number are revised as new sheets are issued. Cumulative compound and numerical indexes are issued every few years.

Publication and Distribution

Selected Infrared Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 2,813 valid sheets in the catalog, of which 2,623 were data sheets; a complete set consists of 7 volumes.

A supplementary publication, "Suggested Procedures Regarding the Arrangement, Filing, and Maintenance of the Loose-Leaf Sheets in the Tables and Spectral Catalogs of the American Petroleum Institute Research Project 44," is available to prospective and current recipients of the sheets. The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

Member companies of the API may receive the data sheets on a subscription basis and may obtain additional sets at a reduced rate. On request, university departments, certain cooperative United States government laboratories, nonprofit institutions, and independent libraries may obtain single sets provided the organization agrees to the payment of (1) an initial set fee of about 10 percent of the normal price for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested may purchase the sheets, in complete sets only, at 30 cents per sheet. Initial sets are completely collated in attractive, durable API binders.

4.2.2. SELECTED INFRARED SPECTRAL DATA (Category B): Manufacturing Chemists Association Research Project

Organization

The Manufacturing Chemists Association (MCA) began to publish infrared spectral data in 1959 as part of its Research Program on Properties of Chemical Compounds. The history of this project is discussed in Section 1.1.3. Bruno J. Zwolinsky, director, Thermodynamics Research Center at Texas A&M University, is in charge of the spectral data program.

Substances

Nonhydrocarbon compounds of defined purity of interest to the chemical industry. Spectra have been issued for organic compounds

containing oxygen, nitrogen, sulfur, halogen, phosphorus, boron, arsenic, sodium, silicon, and zinc, and for boric acid. As the MCA infrared catalog is complementary to that of the American Petroleum Institute, substances covered therein are not duplicated.

Properties

Infrared absorption spectrograms giving percent transmittance versus frequency and wavelength (in general 2 - 15 μ). In addition to the spectral curve, the name, molecular and semistructural formulas of the compound, and the solvent and concentration (if in solution) are given in the legend on the sheet. (Other MCA compilations of data are discussed in Sections 1.1.3., 4.3.2., 4.4.2., 4.5.2., and 4.6.2.)

Sources of Data

Spectra measured in cooperating laboratories (16 as of June 30, 1966). Qualified laboratories may contribute spectra after consultation with the director of the project.

Critical Appraisal

Spectra are selected from those submitted by contributing laboratories, on the basis of the competence of the investigator, the quality of the instrumentation employed, and the purity of the compounds. Currently, emphasis is placed on grating spectra of high resolution. Inferior spectra are replaced as those of greater accuracy with respect to both wavelength and intensity become available. The source and purity of the compound, molecular and semistructural formulas, cell length, and the solvent and concentration (if in solution) are given in the legend. To upgrade quality the project supplies contributors with instructions for use of selected commercial instruments, giving techniques for calibration for absolute wavelengths and intensities.

Currency

Revisions and additions are issued semiannually when warranted by the accumulation of new spectra.

Format

The catalog is made up of 8 1/2" x 11" loose-leaf sheets for which special post binders are available. The sheets are arranged by serial number. Charts from some contributors are linear with respect to wavelength, while others are linear with respect to wave number.

Publication and Distribution

Selected Infrared Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 342 valid sheets of which 302 were data sheets.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

The loose-leaf data sheets are available in complete sets on a gratis basis to all educational institutions of higher learning and certain United States government research laboratories, provided the organization agrees to the payment of (1) an initial set fee of about 10 to 15 percent of the normal cost for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Initial sets are now completely collated in attractive, durable binders. Member companies of MCA and all other industrial organizations may receive the MCA data sheets on a subscription basis. Additional complete sets of loose-leaf data sheets may be purchased at a cost of 30 cents per sheet. Others interested, such as private research institutes, independent libraries, and foreign governments, should contact Texas A&M Data Distribution Office regarding discount subscription rates.

Effective July 1, 1966, the MCA loose-leaf data sheets prepared by the Thermodynamics Research Center, Department of Chemistry, Texas A&M University, will be known as TRC data sheets.

4.2.3. COBLENTZ SOCIETY INFRARED ABSORPTION SPECTRA

Organization

A committee of seven was established in 1957 by the Coblentz Society to expedite the production and distribution of standard reference spectra. The chairman of the committee is Clara D. Smith, Box 152, RD 2, Cranbury, N.J. Permanent address of the Society is

P.O. Box 730, Norwalk, Conn. Spectra are reviewed by competent evaluators and are published by arrangement with the Sadtler Research Laboratories, Inc. (see Section 4.2.7.). A financial return to the Society from the sale of the spectra supports the program.

Substances

Pure compounds and commercial products.

Properties

Infrared absorption spectrograms are issued with percent transmittance plotted against both wavelength in microns and wave number in reciprocal centimeters. For most, the range is 2 - 15 μ but for some it is 2 - 30 μ. The name, empirical or semistructural formula or both, and sometimes values of other properties such as boiling point and refractive index are given with each spectrum.

Sources of Data

Spectra submitted by members of the Society and other investigators.

Critical Appraisal

The collectors check submitted spectra for completeness and consistency of compound or material name and structure, accuracy, and quality. Duplication of existing files may be judged desirable whenever a more useful spectrum is contributed. These spectra are forwarded to a central committee for final labeling, editing, and cross-comparison to ensure publication of the best of the submitted spectra. The long-range goal is a collection of reference spectra of the highest quality.

Format

The collected spectra are published with three curves to an 8 1/2" x 11" page. The source of the spectrum is indicated. Four indexes are

available: alphabetical, molecular formula, chemical classes, and numerical. The Chemical Classes Index each year gives a numerical listing of functional groups with a brief explanation of the type of function included in any group, an alphabetical listing of the functional groups, and a tabular coded listing of all the spectra in the set.

Publication and Distribution

Coblentz Society Spectra, set of 4,000 spectra, 1964, $115 per 1,000. Indexes: Alphabetical Index, Molecular Formula Index, Chemical Classes Index, Numerical Index, $5.00 each, set of four, $10.00.

The spectra are copyrighted by the Coblentz Society but are published and distributed by the Sadtler Research Laboratories, Inc., 1517 Vine St., Philadelphia, Pa. 19102, to whom orders may be sent.

4.2.4. INFRARED SPECTRAL DATA FOR REFERENCE PURPOSES

Organization

A new program has been established within the framework of the American Society for Testing and Materials (ASTM) to collect and critically evaluate reliable infrared spectra, and to index, publish, and distribute them. L. E. Kuentzel, originator of the Wyandotte-ASTM Punched Card Index System under contract with ASTM, directs the program. Supporting funds are received from the Office of Standard Reference Data of the National Bureau of Standards.

Substances

Spectra to be published will be selected from specialized collections that exist in cooperating laboratories and that have not previously been available to the public. Substances of pharmaceutical value will be an important part of the collection, but other groups of industrially important organic substances will be included when justified by number available, quality, and usefulness.

4.2.4.

Properties

Infrared spectra over the range 3,800 - 400 cm^{-1} of quality adequate for identification and analysis purposes. The purity of the compounds will be specified when possible with respect to the type and quantity of any spectroscopically detectable impurity present.

Sources of Data

Governmental, industrial, academic, and other research laboratories that have infrared spectral data collections that can be released and that are of general interest. The spectra will be microfilmed, and enlargements will be made for evaluation and eventual publication. Sources of the spectra will be given when approved by the contributing organization. The spectra collected by the now inactive National Research Council Committee on Spectral Absorption Data (see Section 4.2.8.) are being made available for inclusion in this program.

Critical Appraisal

Spectra to be published under this program will be selected in terms of specifications for Reference Spectra developed by the Coblentz Society, which was commissioned by the Office of Standard Reference Data to develop criteria for evaluation of spectra. The Coblentz Society specifications divide spectra into three categories, Class I, Class II, and Class III. Few, if any, existing spectra meet the rigorous specifications of Class I to be known as Standard Spectra, and they will not be the concern of the ASTM collection.

Class II spectra are obtained with the use of the best currently available spectrophotometers operating at maximum efficiency. The wave numbers as read from the chart should be accurate to ±5 cm^{-1} above 2,000 cm^{-1} and ±3 cm^{-1} below 2,000 cm^{-1}. For publication under Class II, curves from at least two samples obtained from different sources must be available and in reasonable agreement.

Class III spectra are obtained with sufficient accuracy to be useful in the identification of unknown materials. The make and model of the spectrometer used must be reported on the chart, and the dispersing element must be identified (e.g., NaCl prism; grating). Wave-number accuracy should be better than ±30 cm^{-1} at 3,000 cm^{-1} or ±5 cm^{-1}

below 2,000 cm^{-1}. Class III spectra will be accepted for publication only when they are superior to existing published spectra of the same compounds.

The complete text of the Coblentz Society's "Report on Specifications for the Evaluation of Infrared Reference Spectra" is published in Analytical Chemistry, 38, 27A, August 1966.

Currency

Initially most of the spectra will be taken from existing laboratory files and a few from the published literature. Thus complete coverage of the literature is relatively unimportant.

Format

Spectral data sheets will be issued on 8 1/2" x 11" loose-leaf sheets, one spectral curve to a page, and also on 16-mm microfilm. Indexes will be provided by ASTM in their existing program for indexing spectral data (see Section 4.8.1.).

Publication and Distribution

Exact plans for publication and distribution have not been formulated, but it is expected that publication will begin as soon as appropriate blocks of spectra of related chemical compounds become available. The spectra will be obtainable from the American Society for Testing and Materials, 1916 Race St., Philadelphia, Pa. 19103.

4.2.5. DOCUMENTATION OF MOLECULAR SPECTROSCOPY

Organization

Documentation of Molecular Spectroscopy (DMS), established in 1956, is a card system published jointly by Butterworth & Co. (Publishers) Ltd., 88 Kingsway, London, W.C.2, England, and Verlag Chemie, G.m.b.H., Weinheim an der Bergstrasse, West Germany. The data are prepared by well-qualified experts working under the direction of the British DMS Advisory Board, London, and the German Institut

für Spektrochemie und Angewandte Spektroskopie, Dortmund, West Germany. The British Board is headed by H. W. Thompson, Oxford University, and the group at the German institute by H. Kaiser.

Substances

Before 1960, organic substances—pure compounds and natural occurring substances for which the composition had not been established, technical products and mixtures; since 1960, both organic and inorganic substances.

Properties

Infrared absorption spectra within the range 4,000 - 200 cm^{-1} (2.5 - 50 μ) are plotted against percent transmittance and percent absorption. Frequencies of the chief bands and their approximate intensities and peak absorption positions are indicated. Physical properties (melting or boiling point, density, and index of refraction), and molecular and structural formulas are also given. From 4,000 to 2,000 cm^{-1}, the scale is reduced one fourth, allowing sufficient space for the clear presentation of the shorter wavelength range.

Sources of Data

Current literature, previously unpublished spectral data from industrial, governmental, and academic laboratories throughout the world.

Critical Appraisal

Publication of spectra is under the advice and control of an advisory committee consisting of leading spectroscopists. Each spectrum is chosen critically as the best available. The author or source of the spectrum or both, the purity of the substance, and the conditions under which the spectrum was measured are also given. Known errors are called to the attention of subscribers by means of a newsletter sent out at intervals.

Currency

The spectral cards are issued quarterly, approximately 400 cards per set.

Format

DMS spectral traces for organic compounds are reproduced on 5 3/4" x 8 1/4" rose-colored edge-notched cards. The frequencies of the chief brands are listed beside the spectra. A coded classification is notched at the top and at one end of the card. It is based on three structural features: (1) the number of carbon atoms, (2) the basic skeleton, and (3) the substituent groups.

An index to the DMS Card System, the DMS-I-Cards, consists of optical coincidence cards, 5 3/4" x 8 1/4", with a coordination system for 5,000 possible hole spaces in 50 squares subdivided into 100 smaller squares. These cards furnish a means of rapidly obtaining all the spectral cards that have a given property.

Spectral traces for inorganic compounds are reproduced on blue cards similar to the rose-colored cards except that the coding is essentially stoichiometric. Yellow literature cards similar to the spectral cards were issued with Volumes 1 through 6 (24 issues). The cards indicated the author, reference, and an abstract of each article from which a spectrum had been reproduced in addition to other articles of interest, and they were coded with vital data so that reference to the original article was often unnecessary. English and German editions of both the spectral and literature cards were issued giving identical information. Beginning with the 25th issue (Volume 7, 1963), the literature cards have been replaced by a comprehensive literature list of papers on infrared, Raman, and microspectroscopy that have appeared in the same period. This list, printed on punched sheets for insertion in the ring binder provided, is accompanied by a set of IBM sized optical coincidence cards known as the DMS Junior Index. These smaller cards are replaced by a consolidated set of large punched cards every two years. An author index is published yearly.

Publication and Distribution

The DMS card service is obtained by subscription from Butterworth & Co. (Publishers) Ltd., London, W.C.2, England, from Butterworth,

Inc., 7300 Pearl St., Washington, D.C., or from Verlag Chemie, G.m.b.H., Weinheim an der Bergstrasse, West Germany. Volumes 1 through 6 contain 2,000 cards, about 80 percent spectral and 20 percent literature. The spectral cards are supplied slotted or unslotted, the unslotted being marked according to the DMS code. The subscription includes a current literature list in a ring binder, the Junior Index, codes for the literature list, instruction and coding manual for the spectral cards, a formula list for each issue and the newsletters. Literature lists for nuclear magnetic resonance were begun in 1965. The prices for the DMS Spectral and Index cards are as follows:

Cards	Price U.K. (£)	U.S. ($)	W. Germany (DM)
Spectral[a] (volume, each)			
1-4 (unslotted)	67. 0.0.	187.50	750.00
5-8 (unslotted)	75. 0.0.	210.00	840.00
1-4 (slotted)	80. 5.0.	225.00	900.00
5-8 (slotted)	88. 0.0.	247.00	988.00
9- (unslotted)	112.10.0.	315.00	1,260.00
9- (slotted)	130.10.0.	365.00	1,460.00
Index (sets)			
S-1 (1-4999) single	22. 5.0.	62.50	250.00
S-1 (1-4999) multiple	18. 0.0.	50.00	200.00
S-2 (5000-9999) single	26. 5.0.	73.50	295.00
S-2 (5000-9999) multiple	21. 0.0.	59.00	236.00

[a] Each volume consists of four issues, each issue containing about 400 spectral cards (pink) and 100 literature cards (yellow). From Issue 17 (beginning of Vol. 5), spectral cards for inorganic compounds (blue) are included and from Issue 25, the literature cards are replaced by literature lists.

Note: With publication of the last of the 15,000 infrared spectral cards, expected in late 1966, quarterly publication of the cards will be discontinued. The 15,000 cards will serve as a basic analytical tool for research. Certain existing spectra are being replaced as spectra covering a greater range become available, and gaps in the collection are being filled.

4.2.6. THE INFRARED DATA COMMITTEE OF JAPAN

Organization

This committee is a subcommittee of the Infrared and Raman Discussion Group, Tokyo, a joint group formed in 1955 by the Chemical Society of Japan, the Spectroscopical Society of Japan, the Japan Society for Analytical Chemistry, the Pharmaceutical Society of Japan, and the Society of Polymer Science, Japan. The Infrared Data Committee (IRDC) was organized to re-examine the existing infrared data in Japan and to publish an authoritative standard collection of infrared spectra. The Chairman is Professor Takehiko Shimanouchi; Vice-chairmen are Dr. Yo-ichiro Mashiko and Professor Koji Nakanishi. Four additional members of the committee, Yoshio Kitahara, Ichiro Nakagawa, Shin-nosuke Saeki, and Nobuyuki Tanaka, comprise the executive committee.

Substances

Organic compounds with emphasis on newly synthesized substances.

Properties

Infrared spectra in the range 4,000 - 600 cm^{-1} (2.5 - 16.0 μ). The cards also give name of sample, empirical and semistructural formula, molecular weight, melting point, boiling point, refractive index, classification of the substance (e.g., steroid, alkaloid, hydrate), and the type of skeleton (acyclic or type of cyclic). The strongest peak and several weaker peaks are indicated.

Sources of Data

Spectra are measured, using carefully calibrated modern spectrophotometers in three laboratories under the direction of members of the executive committee. The compounds used are obtained from cooperating laboratories, mostly those of universities.

4.2.6.

Critical Appraisal

The spectra are examined and evaluated by members of the committee to insure the publication of authoritative graphs. Care is taken to control the purity of the substance for which spectra are determined. When possible the compounds are purified by gas chromatography.

Units

Percent transmittance is plotted against both wavelength in microns and frequency in reciprocal centimeters.

Currency

Currently, approximately 1,200 cards are issued per year. As of September 1965, 5,000 cards were available.

Format

Spectra are recorded on 5" x 8" specially prepared slotted, edge-notched cards. Wave numbers of absorption bands of greatest intensity are recorded on the spectrogram or marked for punching on the cards. The use of small holes aligned in three rows greatly increases the amount of information derivable from the cards. By a special device the original spectrograms are reduced to card size without distortion. In addition to the spectral data, the date and temperature of measurement, type of spectrophotometer used, serial number, and reference of source are given.

Publication and Distribution

The infrared data cards are published by Nankodo Co., Ltd., Harukicho, Bunkyo-ku, Tokyo, Japan. They are sold on a subscription basis at $238.00 for 1,200 cards (postage included). Asian subscribers receive a special price of $150.00. Export agency is Sanyo Shuppan Bocki Co., Inc., P.O. Box 1705, Tokyo, Central Japan. The agent in the United States is the Preston Technical Abstracts Co., 909 Pitner Ave., Evanston, Ill. 60202. The agent in Europe is Heyden & Son Ltd.,

Spectrum House, Alderton Crescent, Hendon, London, N.W.4, England.

The IRDC Cards are included in the ASTM Spectral Absorption Index (IBM cards) under the code letter "J."

4.2.7. SADTLER STANDARD INFRARED SPECTRA

Organization

The Sadtler Research Laboratories, Inc. was established in 1874 and has issued infrared spectra continuously since 1947. Other Sadtler services include sponsored industrial research, spectral analyses, and a computer service that furnishes a method of locating comparison spectra.

Substances

Pure and commercial organic compounds, the latter including steroids, pyrolyzates, monomers and polymers, agricultural and rubber chemicals, pharmaceuticals, and surface active agents.

Properties

Infrared spectra plotted as percent transmittance versus wavelength in microns (range 2 - 15) and frequency in reciprocal centimeters. The name, molecular and semistructural formula, and boiling point or melting point or both are also given. For a group of 500 substances that cannot conveniently be examined by the usual transmission methods or whose application may prevent convenient transmission study (e.g., films, coatings, and adhesives), attenuated total reflectance (A.T.R.) spectra have been measured. Sadtler also issues ultraviolet and nuclear magnetic resonance spectra (see Sections 4.3.4. and 4.6.3.).

Sources of Data

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

4.2.7.

Critical Appraisal

Spectra are determined in the Sadtler laboratories and are reviewed by consultants. This collection and most other spectroscopic collections suffer from lack of reliable sources of compounds of certified high purity. Sadtler attempts to overcome this problem in part by requesting users to submit results of measurements made on different preparations of compounds found in the Standard Spectra catalog. If the spectra disagree, they are redetermined, and lists of verified spectra are then sent to subscribers.

Currency

Two volumes of 1,000 spectra each are now being issued yearly. As of December 1965, 27,000 spectra had been issued.

Format

"Sadtler Standard Infrared Spectra," a collection of infrared spectrograms of organic compounds that is used for the identification of unknown spectra, formerly published on 5" x 13" cards, is now furnished only on 8 1/2" x 11" sheets, three spectra to a sheet, formerly known as the Midget Edition. A set of standard indexes, and the Sadtler Spec-Finder (a book method of locating infrared spectra by the bands) enable wanted spectra to be located. "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.

Publication and Distribution

Current spectra are purchased on a subscription basis, payable in advance. Prices of infrared spectra publications are as follows:

Standard Infrared Spectra (pure substances)

27 volumes of 1,000 spectra each (complete through 1965), include alphabetical name, molecular formula, chemical classes, numerical, and commercial alphabetical indexes, $3,500.00.

Separate volumes, each $125.00.

Standard Spec-Finder, $50.00.

Indexes purchased separately, set of five, $50.00.

1966 spectra by subscription, includes 2 volumes of 1,000 spectra each, Nos. 27,001 - 29,000, five indexes and Spec-Finder, $350.00.

Standard spectra on 16-mm microfilm, prices same as above.

Binders for Indexes and Spec-Finder, each $5.00.

A pocket-sized booklet of infrared spectra of 26 most common solvents and materials used in infrared laboratories, gratis.

Sadtler Standard Grating Spectra

Publication of 5,000 high-resolution spectra of simple and complex pure organic compounds announced for September 1966. Five volumes or 16-mm roll or cartridge microfilm with Indexes and Grating Spec-Finder, $975.00.

Near Infrared Spectra
Completed set of 2,000 spectra in 9 volumes.*

Far Infrared Spectra
Completed set of 500 spectra in 2 volumes.*

Commercial Spectra
Groups priced separately.*
Commercial Spec-Finder, $25.00.

All spectra are available on microfilm.

Sadtler also provides a lease-buy plan and a rental plan, which may be more economical for some users than an outright purchase. Details concerning these plans are available on request from the publisher.

By special arrangement with the Coblentz Society, Sadtler also publishes "Coblentz Society Spectra" (see Section 4.2.3.).

Published by Sadtler Research Laboratories, Inc., 3316 Spring Garden St., Philadelphia, Pa. 19104.

*Prices available from publisher upon request.

4.2.8. NATIONAL RESEARCH COUNCIL COMMITTEE ON SPECTRAL ABSORPTION DATA

The National Research Council Committee on Spectral Absorption Data, discussed in detail in the first edition of the "Directory of Continuing Numerical Data Projects," was a joint committee of the Division of Physical Sciences and the Division of Chemistry and Chemical Technology. The program under its supervision conducted at the National Bureau of Standards was terminated in 1962. The more than 2,000 compound cards (spectra and properties), and bibliography cards and sheets produced by the project are no longer available for purchase. They are mentioned here because they are of good quality, are still held in many laboratories and libraries, and are referenced in the ASTM indexes of infrared data.

4.2.9. BERKELEY ANALYSIS OF MOLECULAR SPECTRA

Organization

This project at the University of California, Berkeley, has operated under a research grant from the National Science Foundation since February 1959. It owes its existence to an appeal in 1956 to the Joint Commission for Spectroscopy, that a systematic program on the laboratory analysis of the spectra of several important molecules of interest to astrophysicists be initiated. It is now under the joint direction of Sumner P. Davis, Associate Professor of Physics, and John G. Phillips, Professor of Astronomy. Its purpose is to provide as complete analyses as possible of the spectra of selected diatomic molecules.

Substances

Substances upon which a systematic study was planned include CN, C_2, TiO, AlH, NH, BH, MgH, SiH, HgH, SiF, BO, and ZrO. Studies completed or under way include those on CN (red system), HgH, TiO, and C_2 (Swan system).

Properties

For the CN molecule: wavelengths, wave numbers, intensities, and rotational quantum numbers of various branches for the identification of 11,000 lines in 39 bands between λ 4,832 and 11,382 Å.

Sources of Data

The production of spectra and plates to be measured and analyzed is carried out in the Physics Department; the reduction analyses and preparation of the tabular material are performed in the Astronomy Department of the University.

Critical Appraisal

The final results recorded are based upon the measurement of each band on at least two plates. All measures are combined to form the tables. A process of averaging was used for wavelengths, wave numbers, and intensities, the details of the processes being given in the text. The number of arc plates and discharge plates included in each average is indicated under the column heading "Remarks" in the tables. A possible inaccuracy resulting from a line being wider than a sharp single line or being blended with a line of the same or a neighboring band is also indicated. Successful computer programs have been developed to assist in the search for bands in extremely complex spectral regions. These new methods are also applicable to less complicated spectral regions and result in great savings of time and effort.

Currency

To date only the first volume of the series, "The Red System ($A^2\Pi - X^2\Sigma$) of the CN Molecule," has been issued. An informal bi-monthly newsletter reports the progress of the Berkeley Program and related work in other laboratories.

Format

The first publication of the Berkeley Program is a book 8 1/2" x 11". The preface gives a brief history and the purpose of the project, and a 14-page introduction describes the program and explains the procedures used to obtain the recorded data. The remaining 200 pages are tables.

Publication and Distribution

The Red System ($A^2\Pi - X^2\Sigma$) of the CN Molecule, Sumner P. Davis and John G. Phillips, University of California Press, Berkeley and Los Angeles, 1963, x + 214 pp., $9.50.

Forthcoming volumes in the series:

An Analysis of the Spectra of the C_2 Molecule and of the HgH Molecule. Editing for the HgH molecules has been completed and final editing for the C_2 molecule is in progress.

An Analysis of the Spectra of the TiO Molecule.

4.2.10. SPECTRAL DATA AND PHYSICAL CONSTANTS OF ALKALOIDS

Organization

This compilation under the combined editorship of J. Holubek and O. Štrouf of the Research Institute for Natural Drugs, Prague, Czechoslovakia, brings together physical and optical data useful in the identification of alkaloids.

Substances

Alkaloids.

Properties

Infrared and ultraviolet spectrograms are given. The infrared spectra have frequencies in the ranges 2,000 - 700 cm^{-1} and 3,800 - 2,600 cm^{-1}

as abscissa and percent transmission as ordinate. The frequencies of the peaks are tabulated. The ultraviolet spectra have wavelengths in millimicrons as abscissa and log ϵ as ordinate (ϵ is the extinction coefficient).

Molecular and semistructural formulas, melting point, optical rotation, and apparent dissociation constants (in 80 percent aqueous methylcellosolve) expressed as pK are given.

Sources of Data

The spectrograms were recorded in the laboratory of the Research Institute on samples supplied by many workers in the field of alkaloid chemistry to whom credit is given. In most cases, physical constants (melting point and optical rotation) are those supplied by the donors of the samples or from the literature. The pK values have been determined by the authors.

Critical Appraisal

The quality of the spectral data will be consistent since they are recorded on instruments in the Institute. The ultraviolet spectra were measured in methanol with the use of a Zeiss-Jena VSU Universal spectrophotometer (NaCl prism). The infrared spectra of purified samples submitted by collaborators were recorded on a calibrated Zeiss-Jena model UR spectrophotometer. Leading references from the literature regarding the botanical source of individual alkaloids are cited. Synonyms of the alkaloids are cross-referenced in the index.

Currency

Volume I of the compilation contains data on 300 alkaloids. Supplements containing 100 alkaloids each are expected to keep the compilation up to date.

Format

The data are issued on 8 1/2" x 11" cards in post binders. A descriptive introduction, subject index, and bibliography (for

references listed under Occurence)—29 pages in Volume I and 17 pages in Volume II—are printed on lighter-weight paper. A five-page addendum to Volume I is included in the introductory material for Volume II.

Publication and Distribution

Spectral Data and Physical Constants of Alkaloids, J. Holubek and O. Štrouf, eds. Published by Heyden & Sons, Ltd., London, in cooperation with The Publishing House of the Czechoslovakia Academy of Sciences.

Vol. I, 1965, spectral cards 1 - 30 issued in two binders to take Vols. I and II, £23.0.0. ($69.00).

Vol. II, 1966, spectral cards 301 - 400, punched cards to be inserted in second binder, £7.0.0. ($21.00).

Available in Western Europe and the Western Hemisphere from Heyden & Sons, Ltd., Spectrum House, Alderton Crescent, Hendon, London, N.W.4, England.

4.2.11. MICROWAVE SPECTRAL TABLES

Organization

The compilation of this series of tables is being carried out in the Radio Standards Physics Division, Radio Standards Laboratory, National Bureau of Standards (NBS), Boulder, Colo. The tables, now being issued as NBS Monograph 70, are a revision and extension of NBS Circular 518, "Molecular Microwave Spectra Tables," by P. Kisliuk and C. H. Townes, published in 1952 and no longer available. The project is now functioning under the National Standard Reference Data Program of NBS, with Yardley Beers as director of the project. Activity in the field of microwave spectroscopy has increased markedly so that the monograph is being published in five volumes, the first two of which have appeared. Upon completion, the monograph is designed to present a comprehensive compilation of microwave spectra including measured frequencies, assigned molecular species, assigned quantum numbers, and molecular constants determined from these data.

Substances

In Volume I, diatomic molecules for which microwave data are available. In Circular 518, diatomic molecules were a very small fraction of the molecules reported. Volume II tabulates line strengths of asymmetric rotors as a function of Ray's asymmetry parameter κ for rotational quantum numbers J from 0 to 35.

Properties

Spectral lines of diatomic molecules observed by coherent radiation techniques, measured frequencies, assigned molecular species, assigned quantum numbers, and intensities computed for 300° and 195°K; also for each molecule a table of molecular constants such as line widths, rotational constants, dipole moments, and various coupling constants. A separate table lists values of Casimir's function and hyperfine intensities.

Sources of Data

World literature including other compilations of the molecular constants.

Critical Appraisal

Frequencies and uncertainties given are mainly those considered most accurate, but no attempt has been made to reduce uncertainties to a common basis because in many of the original papers they are not precisely defined. When several sources are considered of comparable accuracy, an average of the values is given. In general, the molecular constants are those reported in the original articles. Some intensities were computed without sufficient data to obtain accurate values and are marked "R" for relative. The methods of computation of the intensities are discussed in detail. All computations were carried out on a digital computer, so there are few, if any, random computational errors. Approximations used to simplify the calculations are explained and the constants used are recorded.

The textual material of Volume II defines and discusses line strengths, describes the tables, and gives the procedures for

(1) tabulation and interpolation as a function of κ, (2) extrapolation to higher J values, and (3) method of computation. Accuracy of results is discussed also.

Use of Nomenclature, Symbols, Units, and Physical Constants

The symbols used are defined in the introductory section and are in general agreement with lists of symbols issued by several international committees.

Format

The volumes of NBS Monograph 70 are hard-cover books. In Volume I the spectra and molecular data are ordered alphabetically according to the International Union of Pure and Applied Chemistry names of the compounds. The listing is divided first according to the isotopic molecular species and then according to the major quantum numbers for the transitions. An extensive bibliography lists references numerically, the numbers being assigned first according to year and then alphabetically. References added after the initial numberings are listed according to both numerical and year-author orders. There are 17 pages of textual material followed by 121 pages of tables. Volume II includes 11 pages of textual material and 338 pages of tables.

Publication and Distribution

NBS Monograph 70, Microwave Spectral Tables

Vol. I: Diatomic Molecules, Paul F. Wacker, Masataka Mizushima. Jean D. Peterson, and Joe R. Ballard, Dec. 1, 1964, xviii + 146 pp., 8" x 10 1/2", $2.00.

Vol.II: Line Strengths of Asymmetric Rotors, Paul F. Wacker and Marlene R. Pratto, Dec. 15, 1964, xii + 340 pp., 8" x 10 1/2", $3.00.

Above volumes available from Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

Planned Volumes

Vol. III: Polyatomic Molecules Capable of Internal Rotation.
Vol. IV: Polyatomic Molecules Without Internal Rotation.
Vol. V: Frequency Listing.

4.3. ELECTRONIC SPECTRA (ULTRAVIOLET AND VISIBLE)

4.3.1 SELECTED ULTRAVIOLET SPECTRAL DATA (Category C): American Petroleum Institute Research Project 44

Organization

The American Petroleum Institute (API) Research Project 44, described in Section 1.1.2, began publishing ultraviolet spectral data in 1945. Bruno J. Zwolinski directs the project.

Substances

The catalog is made up mostly of spectra of hydrocarbons; oxygen, halogen, sulfur, and nitrogen derivatives of the hydrocarbons are also included, as well as a few organometallic compounds (particularly etioporphyrins).

Properties

Ultraviolet absorption spectra. The spectral curves give absorbance versus wavelength in ångström units and frequency in reciprocal centimeters, generally in the range 2,100 - 5,300 Å. A table of wavelengths, slit widths, and optical densities (or absorbances) is given on the reverse side of a number of the early sheets. Nominal bandwidths in ångströms are indicated on the charts. Formula and state of the compound being measured are given. (API Research Project 44 also issues physical and thermodynamic data and several other types of spectra. For discussions see Sections 1.1.2, 4.2.1, 4.4.1, 4.5.1, and 4.6.1.).

4.3.1.

Sources of Data

Spectra have been obtained from industrial, academic, governmental, and private laboratories (38 contributing organizations as of June 30, 1966). Qualified laboratories may, after consultation with the project director, submit spectra for inclusion in the catalog.

Critical Appraisal

Spectra are selected from those submitted by the contributing laboratories. Consideration is given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compounds used. The source and purity of the sample, when available, are given in the legend. A policy of replacing inferior old spectra steadily improves the catalog. To upgrade quality, the project supplies contributors with detailed instructions that include recommendations for calibration and techniques to be used in obtaining and recording spectra with a number of acceptable commercial instruments. Operating characteristics are given such as temperature of measurement, cell length, and concentration and solvent if the substance is in solution, or pressures if in the gaseous state.

Currency

Revisions and additions are issued semiannually when warranted by the accumulation of new spectra.

Format

The form of publication is the 8 1/2" x 11" loose-leaf sheet for which special post binders are available. The older spectra are mostly smooth curves redrawn by hand. Most of the spectra issued since 1950 are reduced reproductions of original chart recordings obtained with the Beckman and the Cary spectral photometers on continuous chart paper. Supplemental information is given in the legend. Two indexes are provided, one arranged by type of compound, the other by serial number. Contributing laboratories are identified in the indexes by code letters.

Publication and Distribution

Selected Ultraviolet Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 1,076 valid sheets in the catalog of which 1,069 were data sheets. A complete set consists of 3 volumes.

A supplementary publication, "Suggested Procedures Regarding the Arrangement, Filing, and Maintenance of the Loose-leaf Sheets in the Tables and Spectral Catalogs of the American Petroleum Institute Research Project 44," is available to prospective and current recipients of the sheets. The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

Member companies of API may receive the data sheets on a subscription basis and may obtain additional sets at a reduced rate. On request, university departments, certain cooperative United States government laboratories, nonprofit institutions, and independent libraries may receive single sets provided the organization agrees to the payment of (1) an initial set fee of about 10 percent of the normal price for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested may purchase the sheets, in complete sets only, at 30 cents per sheet. Initial sets are now completely collated in attractive durable API binders.

4.3.2 SELECTED ULTRAVIOLET SPECTRAL DATA (Category C): Manufacturing Chemists Association Research Project

Organization

The Manufacturing Chemists Association (MCA) Research Project, described in Section 1.1.3, began to publish ultraviolet spectral data in 1959. Bruno J. Zwolinski directs the project.

Substances

Emphasis is placed upon inorganic and nonhydrocarbon compounds important to the chemical industry. To date, spectra have been published for organic compounds containing oxygen, nitrogen, sulfur, chlorine, and boron, and for diborane and a number of hydrocarbons.

4.3.2.

Properties

Ultraviolet absorption spectra. The spectral curves give absorbance versus wavelength in ångström units and frequency in reciprocal centimeters, generally in the range 2,100 - 3,700 Å. (For discussions of other compilations of the MCA Research Project, see Sections 1.1.3, 4.2.2, 4.4.2, 4.5.2, and 4.6.2.)

Sources of Data

Spectra measured in cooperating laboratories (seven contributing organizations as of June 30, 1966). Qualified laboratories may, after consultation with the project director, arrange to submit spectra for inclusion in the MCA catalog.

Critical Appraisal

Spectra are selected from those submitted by the contributing laboratories. Consideration is given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compound used. The source, purity of the sample, temperature, cell length, and concentration and solvent if in solution, are stated in the legend. Replacement of old inferior spectra as better ones become available steadily improves the catalog. The project supplies contributors with detailed instructions that include recommendations for calibration and techniques to be used in obtaining and recording spectra with a number of acceptable commercial instruments.

Currency

Revisions and additions are issued semiannually when warranted by the accumulation of spectra.

Format

Publication is in the form of 8 1/2" x 11" loose-leaf sheets for which special post binders are available. The first issue of sheets contains smooth hand-drawn curves whereas the later data sheets are reproductions of chart recordings. The concentrations for various sections

of the spectrogram are indicated on the spectrogram. The sheets are arranged by serial number. Two indexes are provided, one arranged by type of compound and the other by serial number. Contributing laboratories are identified in the indexes by code letters.

Publication and Distribution

Selected Ultraviolet Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 126 valid sheets, of which 103 were data sheets.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

The loose-leaf data sheets are available in complete sets on a gratis basis to all educational institutions of higher learning and certain United States government research laboratories, provided the organization agrees to the payment of (1) an initial set fee of about 10 to 15 percent of the normal cost for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Member companies of MCA and all other industrial organizations may receive the MCA data sheets on a subscription basis. Others interested, such as private research institutes, independent libraries, and foreign governments should contact the Texas A&M Data Distribution Office regarding discount subscription rates. Initial sets are now furnished completely collated in attractive, durable binders. Additional complete sets of loose-leaf data sheets may be purchased at a cost of 30 cents per sheet.

Effective July 1, 1966, the MCA loose-leaf data sheets prepared by the Thermodynamics Research Center, Department of Chemistry, Texas A&M University, will be known as TRC data sheets.

4.3.3. ORGANIC ELECTRONIC SPECTRAL DATA

Organization

Organic Electronic Spectral Data, Inc., is a nonprofit group organized in 1957 by physical-organic chemists concerned about the state of ultraviolet literature. More than 50 chemists from government, industry, and universities searched and abstracted the literature for the first two volumes of data on a volunteer basis.

The organization is quite informal. A treasurer with a five-year term of office provides continuity. Compiling editors, who serve as

officers, are selected for each new volume. Early support came from the publisher, with a grant from the National Science Foundation. Later support has come partly from industry, particularly instrument manufacturers. Processing of the abstract cards for Volumes I, II, and III was carried out at Hebrew University in Jerusalem, Israel, and for Volume IV at the University of Louisville.

Substances

Organic compounds for which spectra have been published in the available journals.

Properties

Wavelength values for maxima, shoulders, and inflections and the logarithms of the corresponding molar absorptivities of ultraviolet and visible spectra are given.

Sources of Data

World literature. For Volumes I and II approximately 65 journals were searched for data, for Volume III, more than 70, and for Volume IV, approximately 90 journals.

Critical Appraisal

The primary purpose of this collection is to aid in compound identification. However, in order to be included, the data have to meet minimum requirements. The compound must be sufficiently pure to permit a satisfactory analysis and be definable by a molecular formula. In general, the solvent, or phase if not in solution, is given. However, some values, marked "n.s.g.," are included if the solvent is not given in the reference paper. The spectral data must be complete enough for the wavelengths of maximal absorption and molar absorptivities to be obtained if they are not given in the original publication. Wavelength values are given to the nearest millimicron unless the original data are given more precisely. Molar absorptivity values are given to the nearest 0.01 unit of log ϵ. Data read from curves are underlined, and the logarithm values are given to 0.1 unit unless the spectrum

enables greater precision to be obtained. Values given to only 0.1 logarithmic unit but not underlined indicate that although numerical values were reported in the original data they were not considered precise enough to warrant the second significant figure after the decimal point. Fine structure at a given maximum is indicated by the letter "f" following the value, and inflections or shoulders are indicated by the letter "s." Coded references are given for all data.

Use of Nomenclature, Symbols, Units, and Physical Constants

The entries are arranged according to the modified Hill (Chemical Abstracts) molecular formula index system. Considerable effort has been made to ensure that the compound names conform with the Chemical Abstracts system of nomenclature, although the application of this policy to the various volumes has been somewhat uneven.

Currency

Volume I, covering the years 1946-1952, and Volume II, the years 1953-1955, were both published in 1961. Volume IV, covering 1958-1959, was published in 1963, and Volume III, covering 1956-1957, in 1966. Volume V, 1960-1961, Volume VI, 1962-1963, and Volume VII, 1964-1965, are in preparation.

Format

The spectral data are presented in 6 1/4" x 9 1/2" bound volumes in four-column tables. The first column lists the compound by formula and name, the second column the solvent, the third column the wavelengths and (log ϵ), and the fourth column the reference. No index is needed because the compounds are arranged according to molecular formula.

Publication and Distribution

Organic Electronic Spectral Data

Vol. I, 1946-1952, M. J. Kamlet, ed., 1961, pp. xiii + 1,244, $25.00.

Vol. II, 1953-1955, H. E. Ungnade, ed., 1960, pp. x + 919, $15.00.

Vol. III, 1956-1957, O. H. Wheeler and L. A. Kaplan, eds., 1966, xii + 1,210 pp., $25.00.

Vol. IV, 1958-1959, J. P. Phillips and F. C. Nachod, eds., 1963, viii + 1,179 pp., $20.00.

Vol. V, 1960-1961, R. E. Lyle and P. R. Jones, eds. (in preparation).

Vol. VI, 1962-1963, L. D. Freedman and J. Cymerman Craig, eds. (in preparation).

Volume VII, 1964-1965, J. C. Dacons and R. G. Rice, eds. (in preparation).

Published by Interscience Publishers, a division of John Wiley & Sons, Inc., New York, London, and Sydney.

4.3.4 SADTLER STANDARD ULTRAVIOLET SPECTRA

Organization

The Sadtler Research Laboratories, discussed in Section 4.2.7, introduced their "Standard Ultraviolet Reference Spectra" in 1960.

Substances

Selection is made from compounds in the Sadtler collection for which ultraviolet spectra will be useful. Pharmaceutical chemicals were the first group of commercial ultraviolet spectra to be included in the collection.

Properties

Ultraviolet absorption spectra in the range 200 - 355 mμ. The molecular and semistructural formula and molecular weight are also given.

Sources of Data

Spectra determined in the Sadtler laboratories on compounds contributed by industrial and research organizations, and educational institutions.

Critical Appraisal

The solvents used in scanning are important, as some bring out better resolution than others. Sadtler makes use of five solvents in an order based on laboratory tests that showed minimum loss of energy with optimum solvent action. The spectra are scanned in acid, base, and neutral media. As many as four absorbancy curves for solutions of various concentrations appear on each chart. The quality of an individual spectrum depends in part on the purity of the compound. Sadtler advertising literature states only that samples at least 98 percent pure are used. No criteria of purity are presented. Each spectrum measured is reviewed by consultants before publication.

The method of preparation for scanning, cell thickness, concentration, wavelength of maximum absorbance, slit opening at this wavelength for each curve, and the instrument used are indicated for each spectrum.

Currency

There were 6,000 spectra issued before 1964, 5,000 in 1964, and 5,000 in 1965.

Format

Photographic copies of the spectra are published, one chart lengthwise on 8 1/2" x 11" loose-leaf sheets. Special binders are available. The indexes to the Sadtler Infrared Spectra are applicable to the ultraviolet reference spectra, but ultraviolet alphabetical and numerical indexes are also published.

Publication and Distribution

The "Sadtler Standard Ultraviolet Spectra" including alphabetical and numerical indexes are available on a subscription basis—$560.00 for the 1965 subscription (5,000 spectra). The 11,000 bound spectra previously issued sell for $1,265.00 including indexes. Individual spectra are priced at 15 cents each. The spectra are also available on 16-mm microfilm at the same price.

Orders and inquiries should be sent to Sadtler Research Laboratories, Inc., 3314-3320 Spring Garden St., Philadelphia, Pa. 19104.

4.3.5 ABSORPTION SPECTRA IN THE ULTRAVIOLET AND VISIBLE REGION

Organization

The compilation "Absorption Spectra in the Ultraviolet and Visible Region" edited by L. Láng is sponsored by the Hungarian Academy of Sciences. The original purpose of the compilers was to add the results of Hungarian research to previous foreign collections and to make available to foreign scientists previously unpublished spectra obtained in Hungary. Since the publication of Volume I, the publications have taken on an international aspect with spectra contributed from other countries (see Sources of Data).

Substances

A wide variety of organic compounds, mostly in solution but a few in the solid or vapor phase, plus a small number of metal complexes and other inorganic substances. It is planned to increase the proportion of medicinal compounds because of the increasing importance of spectroscopy in pharmaceutical research.

Properties

Spectra are represented by graphs of log ϵ (ϵ = extinction coefficient) versus wavelength in millimicrons in the range 200 - 600 mμ and in some cases to 800 mμ. Observed values of log I_0/I from which log ϵ is obtained are tabulated. Data for a given substance are often given in media of different pH as well as in different solvents. In addition, associated data are given: structural and molecular formula, molecular weight, concentration and solvent if in solution, and melting and boiling point.

Sources of Data

All the spectra in Volume 1 were contributed by Hungarian spectroscopists. Volume 2 contains a number of spectra of Polish origin; Volume 3 adds spectra from English and Soviet scientists; Volume 4 adds spectra from Czech authors; and Volume 5 adds spectra from Austria. Most of the spectra have not been published previously. The

number of contributors increased from 21 in Volume 1 to 40 in Volume 4 and 36 in Volume 5. Eight of the original contributors have spectra in either or both Volume 4 and Volume 5 and three of them have spectra in Volume 6.

Critical Appraisal

Spectra and the original measurements, or records, are sent to an editorial board consisting of Dr. Láng and four collaborators, three from institutions in Hungary and one from Poland. Spectra that have been previously published are not included unless additional information is given, such as measurements in different solvents or over a greater range. Melting or boiling points give an indication of purity. Because this compilation is a continuing series, no effort is made to group the spectra according to a particular system. Subject, formula, author, and figure (or diagram) indexes enable the location or absence of a given spectrum to be determined easily. The author index includes the institution with which the author is associated. This information is useful because most of the spectra have not been published elsewhere. The instrument with which measurements were made and length of cell used are indicated. Most of the spectra of Volumes 1 and 2 and a few in the later volumes were obtained with the use of a Beckman Model DU spectrograph. The instruments used for most of the spectra of Volumes 3 - 6 included the Unicam SP 500 and SP 700, Hilger Uvispek, CΦ4, Cary Model 14, Zeiss VSU-1, Zeiss PMQ 11, Jobin-Yvon, Maroc, and Spectromom 201.

Currency

Since publication of Volume 1 in 1959, Volumes 2 - 6 have been published and Volumes 7 and 8 are expected within a year.

Format

This compilation consists of 6 1/2" x 9 3/8" loose-leaf sheets issued in special buckram ring binders. The spectra appear on one side of the sheets on graphs with uniform grids (2.5 cm). The logarithm of ϵ, the extinction coefficient, is plotted as ordinate versus wavelength, in millimicrons, as abscissa. The name and graphic

formula are given on the graph. On the other side of the sheet the supplementary data (see Properties) are given along with the experimental data from which log ϵ is calculated. Although each volume begins on page 1, the spectra are numbered continuously through the volumes (to 1,095 in Volume 6).

A separately bound theoretical and technical introduction accompanies Volume 1. It includes several conversion tables (e.g., wavelengths — wave numbers, wavelengths — fresnels, and a spectroscopical conversion table for energies) and a list of symbols and formulas used in the compilation. The indexes and bibliography for each volume are contained in a small pamphlet that slips into a pocket on the inside of the back cover. The books are in English but the titles of each index are also in German and Russian. Authors and figures are linked together in both the author and figure indexes. Loose-leaf cumulative indexes for Volumes 1 - 5 are included in Volume 5. It is expected that such indexes will be repeated at intervals, probably for every five volumes.

A plastic millimeter grid is included in each volume to increase precision in reading the spectra. Unfortunately the lines do not coincide over an entire figure.

Publication and Distribution

Absorption Spectra in the Ultraviolet and Visible Region (a Theoretical and Technical Introduction), elaborated and edited by Dr. L. Láng; published in German and English in 1959, 2nd edition, 1961, 3rd edition, 1963, 80 pp.

Absorption Spectra in the Ultraviolet and Visible Region, L. Láng, ed.

Vol. 1: Substances, 170, 1959, 414 pp. + Index pamphlet, 24, 2nd edition, 1961, 3rd edition, 1963. Combined introduction and Vol. 1, $18.00.

Vol. 2: Substances, 179, 1961, 408 pp. + Index pamphlet, 31, 2nd edition, 1964, $18.00.

Vol. 3: Substances, 172, 1962, 424 pp. + Index pamphlet, 24, $20.00.

Vol. 4: Substances, 185, 1963, 414 pp. + Index pamphlet, 24, $20.00.

Vol. 5: Substances, 192, 1965, 416 pp. + Index pamphlet, 28. Cumulative Index, Vols. 1 - 5, 1965, 112 pp., $23.00.

Vol. 6: Substances, 197, 1966, 412 pp. + Index pamphlet, 30, $23.00.

Vol. 7: Announced for Nov. 1966.

Vol. 8: Announced for early 1967.

Coproduction of the Academic Press, New York and London, and the Publishing House of the Hungarian Academy of Sciences, Budapest. Printed in English in Hungary. Available in both continents of America from Academic Press, Publishers, 111 Fifth Ave., New York, N.Y. 10003.

4.4. RAMAN SPECTRA

4.4.1. SELECTED RAMAN SPECTRAL DATA (Category D): American Petroleum Institute Research Project 44

Organization

The American Petroleum Institute (API) Research Project 44, described in Section 1.1.2., began to publish Raman spectral data in 1948. Bruno J. Zwolinski directs the project.

Substances

Compounds of interest to the petroleum industry; hydrocarbons, related organic compounds containing oxygen, halogens, sulfur, and nitrogen, and selected organometallic compounds.

Properties

Raman spectra, in the form of photographic or photoelectric chart records. Intensities for Raman shift frequencies are given graphically by wave number (in vacuum) in the range 0 - 4,000 cm^{-1}. Photoelectrically recorded charts are supplemented by tabular presentation of standard intensities for peak values. For some spectra, especially those measured before development of intensity standardization methods, relative intensities are given numerically. Polarization data and line appearance (broad, diffuse, symmetrical, etc.) may be given for photographically recorded spectra. Approximate refractive indexes are included. (Other compilations of API Research Project 44 are discussed in 1.2.1., 4.2.1., 4.3.1., 4.5.1., and 4.6.1.)

4.4.1.

Sources of Data

Spectra measured in cooperating laboratories (12 contributing organizations as of June 30, 1966). Qualified laboratories may submit spectra after consultation with the director of the project.

Critical Appraisal

Spectra are selected from those submitted by contributing laboratories, with consideration given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compounds used. Many recent spectral data sheets give the source and purity (in mole percent) of the compound, the precision of measurement, the exciting line, and operating conditions. Inferior spectra are replaced as better ones become available. To standardize the quality of the spectra, detailed instructions for presentation of data from different types of commercially available instruments are supplied to contributing laboratories. The instructions include recommendations for calibration of the instruments, the determination of standard intensities, and some suggestions for laboratory procedures.

Currency

Revisions and additions are made semiannually when warranted by the accumulation of new spectra.

Format

The form of publication is the 8 1/2" x 11" loose-leaf sheet for which special post binders are available. Before October 1959, spectra were presented in the bar type of chart, with abscissa corresponding to the Raman shifts, and heights indicating the relative intensity. More recent photoelectric recordings are in the form of continuous or semicontinuous curves, with breaks for changes in amplifier sensitivity indicated on the graph. Auxiliary information is given in a legend on the sheets, which are arranged according to serial number. Two indexes are provided, one arranged by type of compound and the other by serial number. The contributing laboratory is identified in the indexes by code letters.

Publication and Distribution

Selected Raman Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 501 valid sheets in the catalog, of which 456 were data sheets. A complete set consists of 2 volumes.

A supplementary publication, "Suggested Procedures Regarding the Arrangement, Filing, and Maintenance of the Loose-leaf Sheets in the Tables and Spectral Catalogs of the American Petroleum Institute Research Project 44," is available to prospective and current recipients of the sheets. The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

Member companies of API may receive the data sheets on a subscription basis and may obtain additional sheets at a reduced rate. On request, university departments, certain cooperative United States government laboratories, nonprofit institutions, and independent libraries may receive single sets provided the organization agrees to the payment of (1) an initial set fee of about 10 percent of the normal price for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested may purchase the sheets, in complete sets only, at 30 cents per sheet. Initial sets are now furnished completely collated in attractive, durable API binders.

4.4.2. SELECTED RAMAN SPECTRAL DATA (Category D): Manufacturing Chemists Association Research Project

Organization

The Manufacturing Chemists Association (MCA) Research Project, described in Section 1.1.3., began to publish spectral data in 1959. Bruno J. Zwolinski directs the programs. The first compilation of Raman spectra was published in 1965.

Substances

Nonhydrocarbon chemical compounds of interest to the chemical industry, such as organic oxygen, halogen, and nitrogen compounds.

4.4.2.

Properties

Raman spectra, in the form of photographic or photoelectric chart records.

Sources of Data

Spectra measured in cooperating laboratories (two contributing organizations as of June 30, 1966). Qualified laboratories may submit spectra after consultation with the director of the project.

Critical Appraisal

Spectra are selected from those submitted by contributing laboratories. The same standards will be adhered to as in the other spectral compilations of MCA. Detailed instructions for presentation of data from different types of instruments are supplied to laboratories contributing data.

Currency

This program began later but parallels the API program. The first set of spectral sheets was published in 1965.

Format

The spectra are published on 8 1/2" x 11" loose-leaf sheets for which special post binders are available. Photoelectric recordings are in the form of continuous or semicontinuous curves, with breaks for changes in amplifier sensitivity indicated on the graph. Auxiliary information is given in a legend on the sheets, which are arranged according to serial number. Two indexes are provided, one arranged by type of compound and the other by serial number. The contributing laboratory is identified in the indexes by code letters.

Publication and Distribution

Selected Raman Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 40 valid sheets in the catalog.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

The loose-leaf data sheets are available in complete sets free to all educational institutions of higher learning and certain United States government research laboratories, provided the organization agrees to the payment of (1) an initial fee of about 10 - 15 percent of the normal cost for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Member companies of MCA and all other industrial organizations may receive the MCA data sheets on a subscription basis. Others interested, such as private research institutes, independent libraries, and foreign governments, should contact the Texas A&M Data Distribution Office regarding discount subscription rates. Initial sets are now furnished completely collated in attractive, durable binders. Additional complete sets of loose-leaf data sheets may be purchased at a cost of 30 cents per sheet.

Effective July 1, 1966, the MCA loose-leaf data sheets prepared by the Thermodynamics Research Center, Department of Chemistry, Texas A&M University, will be known as TRC data sheets.

4.5. MASS SPECTRA

4.5.1. SELECTED MASS SPECTRAL DATA (Category E): American Petroleum Institute Research Project 44

Organization

The American Petroleum Institute (API) Research Project 44, discussed in Section 1.1.1., began to publish mass spectral data in 1947. The only comparable program for the compilation and distribution of mass spectral data is the complementary program of the Manufacturing Chemists Association Project (see Section 4.5.2.). Bruno J. Zwolinski directs both programs.

Substances

Principally hydrocarbons; elemental oxygen, hydrogen, neon, argon, and nitrogen; a few hydrides, oxides, and chlorides; selected organic compounds especially those containing oxygen, halogens, sulfur, and nitrogen.

4.5.1.

Properties

The mass spectral data are presented in tabular form. For each observed mass-to-charge ratio, the relative intensity of the peak and the operating conditions—magnetic field and the ionizing voltage—are given. The type of peak is sometimes indicated. The base peak (with relative intensity of 100), the parent peak and corresponding entries are underscored. The molecular weight, molecular and semi-structural formulas, and approximate boiling point are also given. A matrix or grid format for mass spectral data for hydrocarbons of high molecular weight, introduced in 1961, provides a grid of whole-number mass-to-charge ratios for entry of relative intensities of observed peaks. (This form of presentation emphasizes the relation between peaks that differ in mass units by one CH_2 group.) Relative intensities for fractional ratios and other data are given in the conventional tabular form. (API Research Project 44 also compiles physical and thermodynamic data (see Section 1.1.2.) and several other types of spectra (see Sections 4.2.1., 4.3.1., 4.4.1., and 4.6.1.).

Sources of Data

Spectra received from cooperating laboratories (35 organizations as of June 30, 1966). Qualified laboratories may, after consultation with the project director, submit spectra for inclusion in the catalog.

Critical Appraisal

Spectra are selected from those submitted by the cooperating laboratories, with consideration given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compounds used. The importance of high purity of samples and calibrating gases, including information on isotopic purity, is emphasized. Information concerning the instrument used (make, model, and operating conditions) and the relative intensities and sensitivities for the standards used (n-butane and n-hexadecane) give an indication of the quality of the measurements. To ensure high quality of submitted spectra, instructions, including recommendations for calibration and techniques to be used in the measurements, are provided by the project.

Currency

Revisions and additions are issued semiannually when warranted by the accumulation of new spectra.

Format

The spectra are published on 8 1/2" x 11" loose-leaf sheets for which special post binders are available. The data often extend to the reverse side of the page. Two indexes are provided, one arranged by type of compound and the other by serial number. Spectra in the matrix form are indexed in separate supplements. The name of the contributing laboratory is given on the spectral sheet and identified in the indexes by code letters.

Publication and Distribution

Selected Mass Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 2,342 valid sheets in the catalog, of which 2,191 were data sheets. A complete set consists of 6 volumes.

A supplementary publication, "Suggested Procedures Regarding the Arrangement, Filing, and Maintenance of the Loose-leaf Sheets in the Tables and Spectral Catalogs of the American Petroleum Institute Research Project 44," is available to prospective and current recipients of the sheets. The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

Member companies of API may receive the data sheets on a subscription basis and may obtain additional sets at a reduced rate. On request, university departments, certain cooperative United States government laboratories, nonprofit institutions, and independent libraries may receive single sets provided the organization agrees to (1) the payment of an initial set fee of about 10 percent of the normal price for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested may purchase the sheets, in complete sets only, at 30 cents per sheet. Initial sets are now furnished completely collated in attractive, durable API binders.

4.5.2. SELECTED MASS SPECTRAL DATA (Category E): Manufacturing Chemists Association Research Project

Organization

The Manfacturing Chemists Association (MCA) Research Project, described in Section 1.1.3., began to publish mass spectral data in 1959. Bruno J. Zwolinski is in charge of the program.

Substances

In general, nonhydrocarbon compounds containing oxygen, halogens, sulfur, nitrogen, silicon, and boron; some hydrocarbons; hydrides of boron, bromine, and silicon. High-quality spectra of any compounds not included in the American Petroleum Institute catalog are accepted. Duplication in the two catalogs is avoided.

Properties

The mass spectral data are present in tabular form. For each observed mass-to-charge ratio, the relative intensity of the peak and the operating conditions—magnetic field and ionizing voltage—are given. The type of peak is sometimes indicated. The base peak (with relative intensity of 100), the parent peak and corresponding entries are underscored. The molecular weight, molecular and semistructural formula, and approximate boiling point of the compound are also given. MCA also compiles and publishes physical and thermodynamic data (see Section 1.1.3.) and several other types of spectra (see Sections 4.2.2., 4.3.2., 4.4.2., and 4.6.2.).

Sources of Data

Spectra received from cooperating laboratories (five organizations as of June 30, 1966). Qualified laboratories may, after consultation with the project director, submit spectra for inclusion in the catalog.

Critical Appraisal

Spectra are selected from those submitted by the cooperating laboratories, with consideration given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compounds. Older spectra are systematically replaced by improved spectra as they become available. The importance of high purity of samples and calibrating gases, including information on isotopic purity, is emphasized by the project. Information concerning the instrument used (make, model, and operating conditions) and the relative intensities and sensitivities for the standards (n-butane and n-hexadecane) give an indication of the quality of the measurements. To ensure high quality of submitted spectra, instructions including recommendations for calibration and techniques to be used in the measurements are provided by the project. Corrections and instrument modifications or conditions that affect the quality of the data are sometimes recorded.

Currency

Revisions and additions are issued semiannually when warranted by the accumulation of spectra.

Format

Publication is in the form of 8 1/2" x 11" loose-leaf sheets for which special post binders are available. The tabular data often extend to the reverse side of the page. (In 1961 a new matrix or grid format for mass spectral data for hydrocarbons of high molecular weight, described in Section 4.5.1., was made available. To date, this form has not been used by contributors to the MCA Mass Spectral Data.) Two indexes are provided, one arranged by type of compound and the other by serial number. The name of the contributing laboratory is given on the spectral sheet and identified in the index by code letters.

Publication and Distribution

Selected Mass Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 168 valid sheets in the catalog.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

The loose-leaf data sheets are available in complete sets free to all educational institutions of higher learning and certain United States government research laboratories, provided the organization agrees to the payment of (1) an initial set fee of about 10 - 15 percent of the normal cost for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Initial sets are now furnished completely collated in attractive, durable binders. Additional complete sets of loose-leaf data sheets may be purchased at a cost of 30 cents per sheet. Member companies of the MCA and all other industrial organizations may receive the MCA data sheets on a subscription basis. Others interested such as private research institutes, independent libraries, and foreign governments should contact the Texas A&M Data Distribution Office regarding discount subscription rates.

Effective July 1, 1966, the MCA loose-leaf data sheets prepared by the Thermodynamics Research Center, Department of Chemistry, Texas A&M University, will be known as TRC data sheets.

4.5.3. COMPILATION OF MASS SPECTRAL DATA (INDEX DE SPECTRES DE MASSE)

Note. This publication, because it is more than an index, is discussed briefly here. It was first published in the form of four paper-backed volumes by the Commissariat à L'Énergie Atomique. Sections A, B, and C of the Heyden edition are arranged as in the earlier publication, but Section D replaces a volume arranged in the order of the highest peaks of the substances.

"Compilation of Mass Spectral Data" by A. Cornu and R. Massot is a four-part index to a collection of about 5,000 spectra (mostly of organic compounds) maintained at the Laboratory of Mass Spectrometry, Centre of Nuclear Studies, Grenoble, France, under the Commissariat à L'Énergie Atomique. Each part lists the name of the element or compound, the reference, the molecular weight, a number for calculating absolute peak heights from that of a standard, the ten highest peaks and their relative abundances (or intensities), and the formula (given by listing the number of atoms under each element present). The parts are arranged in four ways, Section A by reference numbers to compilations of mass spectra (identified in the introduction), Section B by molecular weight, Section C by molecular formula, and Section D by fragment ion values (including the molecular ion). Parts

A, B, and C each have 98 pages, but Part D, because it lists fragments, has 323 pages. The identification of a substance may often be determined without access to its complete spectrum but, if it is needed, the reference enables it to be found.

Publication and Distribution

Compilation of Mass Spectral Data (Index de Spectres de Masse), A. Cornu and R. Massot, 1966, xv + 617 pp., 8 1/2" x 11". Published by Heyden & Sons Ltd., in cooperation with Presses Universitaires de France. Distributed by Heyden & Sons Ltd., Spectrum House, Alderton Crescent, London, N.W.4, England; $42.00.

4.6. NUCLEAR MAGNETIC RESONANCE SPECTRA

4.6.1. SELECTED NUCLEAR MAGNETIC RESONANCE SPECTRAL DATA (Category F): American Petroleum Institute Research Project 44

Organization

The American Petroleum Institute (API) Research Project 44, discussed in Section 1.1.2., began to publish nuclear magnetic resonance (NMR) spectra in October 1959. Bruno J. Zwolinski directs the program.

Substances

Mostly hydrocarbons and related organic compounds containing oxygen, nitrogen, and sulfur; a few organometallic compounds of interest to the petroleum industry.

Properties

NMR spectra. The spectral data are presented as reduced reproductions of instrument tracings. The standard abscissa scale is frequency separation (in cycles per second) from the external reference

standard, although secondary scales are frequently employed, such as the shielding numbers, N for external references, τ for internal references. The abscissa scale for the more recent sheets is in parts per million. The height of each resonance peak is normally shown without scale, and the exact frequencies of prominent resonances are usually identified on the spectrum. (Other compilations of API Research Project 44 are discussed in Sections 1.1.2., 4.2.1., 4.3.1., 4.4.1., and 4.5.1.)

Sources of Data

Cooperating laboratories (14 organizations as of June 30, 1966). Qualified laboratories may make contributions, after consultation with the director of Research Project 44.

Critical Appraisal

Spectra are selected from those submitted by contributing laboratories, with consideration given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compounds. Inferior spectra are replaced as better ones become available. API Standard or Research Samples are used in many of the measurements. Information is generally given concerning purity, source of compound, identification of external reference standard, instrument used, and operating conditions. The project supplies contributors with instructions that encourage the use of both internal and external reference standards, describe standardization methods, and provide useful suggestions on experimental techniques.

Currency

Revisions and additions are issued semiannually.

Format

Publication is in the form of 8 1/2" x 11" loose-leaf sheets for which special post binders are available. The spectra, sometimes including multiple curves at different scanning rates, are shown graphically,

usually with two abscissa scales. Supplementary information is given in a legend. Sheets are arranged according to serial number. Indexed include a numerical listing by serial number, a formula index subdivded by chemical classes of compounds, and a functional group index arranged alphabetically. The Functional Group Index lists 253 NMR (40-megacycle) spectral data sheets contributed by the Humble Oil and Refining Company. Of these, 103 are in the API Research Project 44 Catalog and 150 in the MCA Research Project Catalog.

Publication and Distribution

Selected Nuclear Magnetic Resonance Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 649 valid sheets in the catalog, of which 583 were data sheets. A complete set consists of 2 volumes.

A supplementary publication, "Suggested Procedures Regarding the Arrangement, Filing, and Maintenance of the Loose-leaf Sheets in the Tables and Spectral Catalogs of the American Petroleum Institute Research Project 44," is available to prospective and current recipients of the sheets. The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

Member companies of API may receive the data sheets on a subscription basis and may obtain additional sets at a reduced rate. On request, university departments, certain cooperative United States government laboratories, nonprofit institutions, and independent libraries may receive single sets provided the organization agrees to the payment of (1) an initial set fee of about 10 percent of the normal price for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Others interested may purchase the sheets, in complete sets only, at 30 cents per sheet. Initial sets are now furnished completely collated in attractive, durable API binders.

4.6.2. SELECTED NUCLEAR MAGNETIC RESONANCE SPECTRAL DATA (Category F): Manufacturing Chemists Association Research Project

Organization

The Manufacturing Chemists Association (MCA) Research Project established in 1955, described in Section 1.1.3., began to publish

nuclear magnetic resonance (NMR) spectra in December 1960. Bruno J. Zwolinski directs the project.

Substances

Nonhydrocarbon compounds: to date, organic compounds containing oxygen, halogen, sulfur, nitrogen, and phosphorus have been treated.

Properties

NMR spectra. The data are presented as reduced reproductions of instrument tracings. The standard abscissa scale is frequency separation (in cycles per second) from benzene, the external reference standard; for a few, it is parts per million, and for some both units are given. The shielding number is usually given as a secondary horizontal scale. The height of resonance peaks is normally shown without scale. Exact frequencies of prominent resonances are identified on the spectrum. (Other compilations of MCA are discussed in Sections 1.1.3., 4.2.2., 4.3.2., 4.4.2., and 4.5.2.)

Sources of Data

Spectra measured in cooperating laboratories (eight contributors as of June 30, 1966). Qualified laboratories may submit spectra, after consultation with the director of the project.

Critical Appraisal

Spectra are selected from those submitted by contributing laboratories, with consideration given to the competence of the investigator, the quality of instrumentation employed, and the purity of the compounds. Inferior spectra are replaced as better ones become available. For some of the samples, the source and purity of the material are given. The project supplies contributors with instructions that encourage the use of both internal and external reference standards, describe standardization methods, and provide useful suggestions on experimental techniques.

Currency

Revisions and additions are issued semiannually.

Format

Publication is in the form of 8 1/2" x 11" loose-leaf sheets for which special post binders are available. The spectra, sometimes including multiple curves at different scanning rates, are shown graphically, usually with two abscissa scales. Sheets are arranged according to serial number. Indexes include a numerical listing by serial number, a formula index subdivided by chemical classes of compounds, and a functional group index arranged alphabetically. The Functional Group Index includes 253 NMR (40-megacycle) spectral data sheets contributed by the Humble Oil and Refining Company. Of these, 103 are in the API Research Project 44 Catalog and 150 in the MCA Catalog.

Publication and Distribution

Selected Nuclear Magnetic Resonance Spectral Data, current loose-leaf sheets. As of June 30, 1966, there were 551 valid sheets in the catalog, of which 492 were data sheets. A complete set consists of 2 volumes.

The data sheets are distributed by the Data Distribution Office, Texas A&M Research Foundation, College Station, Texas.

The loose-leaf data sheets are available in complete sets free to all educational institutions of higher learning and certain United States government research laboratories, provided the organization agrees to the payment of (1) an initial set fee of about 10 - 15 percent of the normal cost for back issues, and (2) a handling charge of 10 cents per sheet for all current semiannual supplements issued. Initial sets are now furnished completely collated in attractive, durable binders. Additional complete sets of loose-leaf data sheets may be purchased at a cost of 30 cents per sheet. Member companies of MCA and all other industrial organizations may receive the MCA data sheets on a subscription basis. Others interested, such as private research institutes, independent libraries, and foreign governments should contact the Texas A&M Data Distribution Office regarding discount subscription rates.

Effective July 1, 1966, the MCA loose-leaf data sheets prepared by the Thermodynamics Research Center, Department of Chemistry, Texas A&M University, will be known as TRC data sheets.

4.6.3. SADTLER NUCLEAR MAGNETIC RESONANCE SPECTRA

Organization

The Sadtler Research Laboratories, discussed in Section 4.2.7., began to issue Nuclear Magnetic Resonance (NMR) spectra in 1964.

Substances

Selected compounds for which NMR spectra will be useful and for which Sadtler Infrared Standard Spectra are available.

Properties

NMR spectra presented as reproductions of instrument tracings with the abscissa as a dual scale in parts per million and cycles per second. Semistructural formulas are given with the assignments indicated on the formulas as well as tabulated. Molecular weight, melting and boiling points (when known), and sometimes index of refraction are also given.

Sources of Data

All spectra determined in the Sadtler laboratories.

Critical Appraisal

The spectra are scanned with a Varian A-60 High Resolution NMR spectrometer. Appropriate solvents such as deuterated chloroform are used. Tetramethylsilane is used as an internal reference. The sweep offset, frequency response, sweep time, spectrum amplitude, weight of sample per volume of $CDCl_3$, and asssignments are recorded. The source of the compound and when applicable the number of the corresponding Sadtler infrared spectrum are given so that identification of an unknown sample may be made more easily. Alphabetical, numerical, and molecular formula indexes are provided to make the spectra easily accessible.

Currency

The first subscription consists of 2,000 NMR spectra. Plans for future releases have not been announced.

Format

The spectra are issued on 8 1/2" x 11" sheets (two spectra with consecutive numbers to a page) and on 16-mm microfilm in cartridge or roll form. The sheets are contained in a vinyl loose-leaf binder.

Publication and Distribution

The Sadtler NMR spectra are available on a subscription basis with shipments made at irregular intervals.

First issue, 2,000 NMR spectra with indexes: prepublication price, bound sheets or microfilm, $300.00 f.o.b., Philadelphia, Pa. Later price, $500.00.

Orders and enquiries should be sent to Sadtler Research Laboratories, Inc., 3316 Spring Garden St., Philadelphia, Pa. 19104.

4.6.4. HIGH RESOLUTION NUCLEAR MAGNETIC RESONANCE SPECTRA

Organization

Two catalogs of high resolution Nuclear Magnetic Resonance (NMR) spectra have been prepared by members of the Instrument Division of Varian Associates, Palo Alto, Calif. The object was to supply a carefully selected set of NMR spectra that would (1) fill the need of chemists attempting to interpret high resolution spectra, and (2) lay the groundwork for interpreting mixtures encountered in analytical work.

Substances

Compounds for which the following criteria are met: (1) a spectrum that includes several interpretable chemical shift positions character-

istic of functional groups frequently encountered in organic structure problems, (2) presence of more than a single line with interpretable fine structure illustrating either a chemical shift or spin-spin coupling pattern, and (3) availability of a sufficiently pure sample. Among the substances included are alkaloids, monomers, peroxides, steroids, terpenes, and vitamins.

Properties

NMR spectra presented as reproductions of instrument tracings with the abscissa as a dual scale in parts per million (δ) and cycles per second. Semistructural formulas are given with the assignments indicated on the formulas and their values tabulated.

Sources of Data

All spectra obtained in the Applications Laboratory of the Instrument Division of Varian Associates.

Critical Appraisal

The instrument used was the Varian A-60 High-Resolution NMR Spectrometer. The calibration of the instrument was checked frequently and all data were believed by the authors to be within 1 cps or 0.02 ppm. The sweep offset, sweep time, frequency response, specific instrument amplitude setting, and unusual operating conditions are given. An alphanumeric system of coding proton chemical environments was set up to permit a search of the functional group contents of the spectra in the collection. The system, based upon main, sub, and sub-sub groups, is fully described, and examples of the coding are given. Three indexes—name, functional group, and chemical shift—simplify the location of a spectrum. In some cases in Volume II, a 100-mc trace is included above the 60-mc trace to aid in interpreting the spectrum. Also, proton-proton spin decoupling has been used to verify some of the spectral assignments and is so indicated in the title block.

The solvent used for the spectra in Volume I was deuterated chloroform, and the internal reference was tetramethylsilane; for Volume II, the solvent was D_2O or D_2O (NaOD) and the reference sodium 2,2-dimethyl-2-silapentane-5 sulfonate (DSS) dissolved in the solution.

Currency

These volumes make no effort to cover all spectra recorded in the literature. In 1962, when Volume I was published, approximately 350 spectra were considered sufficient for the stated purpose but since many important types of proton chemical environment were not included and the response to Volume I had been favorable, a second volume was issued in 1963.

Format

The catalogs are soft-cover, spiral bound loose-leaf sheets, 8 1/2" x 11", with two spectra per page. The preface to Volume I appears in both volumes and describes the compilation and its use. A second preface in Volume II calls attention to the differences in the two volumes. The indexes in Volume II are cumulative for the two volumes. A foldout chart of the main and functional groups on the last page of each volume is an aid in assigning structure to a compound.

Publication and Distribution

High Resolution NMR Spectra Catalog, Vol. I, 1962, N. S. Bhacca, L. F. Johnson, and J. N. Shoolery, compilers, 43 pp. + 368 spectra, $6.00; 10 or more copies, $4.50 each; student price, $5.00.

High Resolution NMR Spectra Catalog, Vol. II, 1963, N. S. Bhacca, D. P. Hollis, L. F. Johnson, and E. A. Pier, compilers, x + 62 pp. + 332 spectra; price same as Vol. I; combined edition, Vols. I and II, hard cover, $20.00.

Available from Varian Associates, Instrument Division, Palo Alto, Calif. 94303.

4.7. OTHER ATOMIC AND MOLECULAR PROJECTS

4.7.1. INTERATOMIC DISTANCES AND CONFIGURATIONS IN MOLECULES AND IONS

Organization

This publication is the outgrowth of a 26-page compilation by P. W. Allen and L. E. Sutton in Acta Crystallographica, 3, 46, 1949. Con-

sideration of the need for a more comprehensive work resulted in a cooperative compilation by specialists with the advice and help of a number of other specialists. The main volume was sponsored by The Chemical Society, London, and issued as their special Publication No. 11 in 1959. Financial assistance, in the way of an advance purchase, was given by the European Research Office of the Department of the United States Army. A supplement, upon which work began in 1959, was supported entirely by The Chemical Society, London, and appeared as their Special Publication No. 18 in 1965. L. E. Sutton was the scientific editor of both volumes. It is understood that work is continuing with the expectation of publishing a second edition or supplement.

Substances

Most elements and their compounds or ions for which interatomic distances and bond angles have been measured; gaseous molecules or radicals; molecules in the solid state; complex ions occurring in a solid; crystals for which pairs of ions have been reported as molecules or ion-pairs in the vapor state; and adamantine lattices. The emphasis is on molecules, no attempt having been made to cover minerals, salts, or alloys. Both inorganic and organic compounds are included.

Properties

Interatomic distances, bond angles, crystal structure, molecular formulas with perspective diagrams showing spatial arrangement when needed, and crystallographic symmetry in both the Hermann-Maugium and Schoenflies notations.

Sources of Data

Mostly journal articles, some books.

Critical Appraisal

Data were obtained from spectroscopic, electron diffraction, neutron diffraction, and x-ray diffraction measurements. For vapor-phase measurements, preliminary results are included unless they have been superseded by later work at the same institution. A few unpublished data have been included. For data from papers published in Japanese, the compilers had to rely upon abstracts (provided by the Japanese authors or published in Chemical Abstracts). References for electron diffraction data are more comprehensive than for other subjects. For early crystallographic work other compilations are cited. If an author corrected an earlier paper, only the later reference is given. In the supplement, values for data published in final form since 1955 are recorded only if a change has been made in those reported in the main volume. Both references are given with the notation that the later supersedes the earlier one. Thus, it is often necessary to consult both the main volume and the supplement. In both volumes, coded references, which include date and method of measurement, often make possible a quick guess as to the reliability of the values quoted. Complete references are also given for each entry in the supplement. Bond lengths and angles obtained from crystalline structure are graded in three classes. In general, the results of the top grade, marked with two asterisks, are considered reliable within ±0.02 Å or better and the middle grade, marked with one asterisk, reliable within ±0.05 Å. The third grade is marked "errors uncertain," but the errors are unlikely to exceed ±0.1 Å. Preliminary or doubtful results and comments made or values recalculated by the compiler are indicated. Notations, formulas, diagrams, and symmetry symbols are fully explained in the detailed introduction. The Supplement includes lists of errata in and addenda to the main volume.

Use of Symbols and Units

All symbols are adequately explained. Values for bond lengths are given in ångström units, angles in degrees of arc.

Currency

For the 1958 edition, the literature was searched through 1955, but a few later data are included. The Supplement covers the period 1956 through 1959 as completely as possible and again includes a few later data.

Format

Publication is in 7" x 9 3/4" books. The main volume consists of a preface, a short guide to the tables, a comprehensive introduction, a 19-page table of selected bond lengths, the main table of 259 pages (101 of which are devoted to inorganic compounds and 158 to organic compounds), a 69-page reference table, and a 9-page classified name index. The supplement follows the same pattern and includes a 208-page supplementary main table and 33 pages of additional references. Pagination of both volumes is by sections. The references are listed according to year, journal, method, and serial number. Section A (inorganic) of the main table is arranged according to the Mendeléeff classification of elements, compounds being listed under the most electropositive element (except hydrogen). Section B (organic) follows the Chemical Abstracts system of arrangement.

Publication and Distribution

Tables of Interatomic Distances and Configuration in Molecules and Ions, L. E. Sutton, scientific ed., Special Publication 11, 1958, 390 pp., £2.2.0. ($6.00).

Tables of Interatomic Distances and Configuration in Molecules and Ions, Supplement, 1956 - 1959, L. E. Sutton, scientific ed., Special Publication 18, 1965, 296 pp., £4.4.0. ($12.00).

Published by The Chemical Society, Burlington House, London, W.1, England. Also available from Polycrystal Book Service, P. O. Box 11567, Pittsburgh, Pa. 15238.

4.8. INDEXES

4.8.1. INDEXES TO INFRARED SPECTRAL DATA COMPILATIONS

The American Society for Testing and Materials (ASTM) publishes indexes "a" through "e." They include references to most of the above compilations in addition to some collected from the literature by cooperating committees. For ASTM address, see Section 2.4.1.

a. Infrared Spectral Index Cards, Wyandotte-ASTM, DS32 and Supplements DS32-S1 to DS32-S12, a total of 75,083 standard IBM cards: members, $1,500.00, nonmembers, $2,140.00.

Infrared Spectral Indexes are available on computer tapes for IBM 7090, 7094, 1401, and Honeywell-400 computers. Write ASTM for details.

b. ASTM Infrared Optical Coincidence Index Cards, DS31

Deck A: Peaks present ±0.1 micron (odd)—69 cards; peaks absent 0.3 micron range—46 cards.

Deck B: Sample state, elements, functional groups—39 cards.

Deck C: Peaks present ±0.1 micron (even)—70 cards.

Deck A: Members, $345.00; nonmembers, $402.50.
Decks A & B: Members, $462.00; nonmembers, $539.00.
Decks A, B, & C: Members, $672.00; nonmembers, $784.00.

c. Infrared Molecular Formula—Name Index Cards, Wyandotte-ASTM (Standard IBM cards); DS33, with supplements. Write ASTM for details.

d. Infrared Molecular Formula List of Compounds, Names, and References to Published Infrared Spectra, designed principally for users of the Wyandotte-ASTM system but serves as a source of published literature of infrared spectra.

Issued as ASTM - STP 331, 1962, 316 pp., paper cover. Number changed to DS24 (1965): members, $8.00, nonmembers, $10.00; first supplement, DS24-S1, 1963: 112 pp., members, $3.15, nonmembers, $4.50.

e. Serial Number List of Compound Names and References to Published Infrared Spectra (STP 358), DS29, 1963, 438 pp., hard cover: members, $8.40, nonmembers, $12.00.

f. Documentation of Molecular Spectroscopy issues DMS Index Cards. They are described in Section 4.2.5.

4.8.2. INDEXES TO ULTRAVIOLET - VISIBLE SPECTRAL DATA COMPILATIONS

The American Society for Testing and Materials (ASTM) publishes the following indexes. For ASTM address, see Section 2.4.1.

a. Ultraviolet and Visible Spectral Absorption Index Cards, ASTM-Wyandotte, DS34 and Supplements DS34-S1 to DS34-S6, a total of 18,102 standard IBM cards including 1,500 relating to spectra in the visible light range. Write ASTM for details.

b. Ultraviolet-Visible Molecular Formula—Name Index Cards, Wyandotte-ASTM, DS35 includes Supplements 1 and 2; third supplement DS35-S3 and fourth supplement DS35-S4; 26,337 IBM cards including those in the four supplements. Write ASTM for details.

c. Molecular Formula List of Compound Names and References to Published Ultraviolet and Visible Spectra, a listing of 16,130 compounds of spectra in the Wyandotte-ASTM system through its fifth supplement, 1963, 154 pp. (STP-357), DS28, hard cover: members, $4.20, nonmembers, $6.00.

4.8.3. INDEXES TO MASS SPECTRAL DATA COMPILATIONS

The American Society for Testing and Materials (ASTM) publishes "a" and "b" of the following indexes. For ASTM address, see Section 2.4.1.

a. Index of Mass Spectral Data, an index of approximately 3,200 mass spectra; five separate indexes based on molecular weight, most intense peak, second peak, third peak, and fourth peak, 1964, 248 pp. (STP-356), DS27, hard cover: members, $13.00, nonmembers, $18.50.

b. Mass Spectral Data—Punched Card Index, Wyandotte-ASTM, Mass Spectral Data, 3,200 cards, DS27-1a, $96.00; Mass Spectral Name Formula, 3,500 cards, DS27-1b, $115.00; members, 30% discount.

c. Compilation of Mass Spectral Data (Index de Spectres de Masse), A. Cornu and R. Massot. See Section 4.5.3.

5
Comprehensive Projects

5.1. LANDOLT- BÖRNSTEIN

Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik, und Technik; and Zahlenwerte und Funktionen aus Naturwissenschaften und Technik—Neue Serie (Numerical Data and Functional Relationships in Science and Technology—New Series).

Organization

In 1883, Hans Landolt, with the collaboration of Richard Börnstein, issued the first (one volume) edition of "Physikalisch-Chemische Tabellen." Work on the sixth edition of Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik, und Technik," 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 H. Borchers, H. Hausen, K. H. Hellwege, Kl. Schäfer, E. Schmidt, and the late J. Bartels. The rapid advance in existing fields of physical science and the growth of important new fields made it evident that after publication of the sixth edition it would be practically impossible to resume publishing with such a comprehensive coverage of all fields of science. Beginning in 1961,

publication of a new series of volumes was started. These volumes will appear under the general title "Numerical Data and Functional Relationships in Science and Technology" and are, at present, under the general editorship of K. H. Hellwege. The selection of topics for this series is determined by the current trends and needs of science. Thus active fields will be the subject of frequently published volumes, and inactive fields may receive no attention for many years.

Substances

Very wide coverage including elements (all nuclides), organic and inorganic compounds, and characterized systems of compounds as necessitated by the contents of the individual volumes.

Properties

The goal of the editors of the sixth edition has been to present comprehensively all the important fundamental properties of physics, chemistry, astronomy, geophysics, and technology. In the new series an entire volume may be devoted to a limited area of research.

Source of Data

World literature. The lists of references are very complete and provide a useful guide to the literature in specific fields.

Critical Appraisal

Data for the sixth edition have been more critically examined than those in previous editions. There is no over-all standard by which data are evaluated, the standard for each volume depending upon the individual compilers and editors.

Currency

All the volumes of a compilation with publication extending over more than 15 years cannot possibly be current. The establishment of the new series is an attempt to bring the earlier volumes of the sixth

edition up to date in the most important areas and to present data in new fields of interest.

Format

The volumes of the sixth edition are published as 8" × 10 7/8" cloth-bound books, divided into sections. The individual volumes have no indexes, but an index for the entire sixth edition is in preparation. A table of contents is given in each book, with the applicable part repeated at the beginning of each section in some of the volumes. Data are presented in tables and graphs. References either accompany the individual tables or graphs, or are placed at the end of the section. Earlier editions and most volumes of the sixth edition are in German. A welcome trend evident in some recent volumes, and planned for all volumes of the new series, is to have the introductory material and a large part of the data and explanatory paragraphs in both German and English.

Publication and Distribution

Landolt-Börnstein: Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik, sixth edition.

Volumes Published

Vol. I: Atom- und Molekularphysik

Part 1, Atome und Ionen, 1950, xii + 441 pp., DM 126 ($31.50).
Part 2, Molekeln I: Kerngerüst, 1951, viii + 571 pp., DM 168 ($42.00).
Part 3, Molekeln II: Elektronenhülle, 1951, xi + 724 pp., DM 218 ($54.50).
Part 4, Kristalle, 1955, xi + 1,007 pp., DM 318 ($79.50).
Part 5, Atomkerne und Elementarteilchen, 1952, viii + 470 pp., DM 148 ($37.00).

Vol. II: Eigenschaften der Materie in Ihren Aggregatzuständen

Part 2, Gleichgewichte ausser Schmelzgleichgewichten.
2a, Gleichgewichte Dampf-Kondensat und Osmotische Phänomene, 1960, xi + 974 pp., DM 448 ($112.00).
2b, Lösungsgleichgewichte I, 1962, x + 983 pp., DM 510 ($127.50).
2c, Lösungsgleichgewichte II, 1964, viii + 731 pp., DM 403.5 ($100.88).
Part 3, Schmelzgleichgewichte und Grenzflächenerscheinungen, 1956, xi + 535 pp., DM 198 ($49.50).

Part 4, Kalorische Zustandsgrössen, 1961, xii + 863 pp., DM 438 ($109.50).
Part 6, Elektrische Eigenschaften I, 1959, xv + 1,018 pp., DM 448 ($112.00).
Part 7, Elektrische Eigenschaften II, 1960, xii + 959 pp., DM 478 ($119.50).
Part 8, Optische Konstanten, 1962, xv + 901 pp., DM 476 ($119.00).
Part 9, Magnetische Eigenschaften I, 1962, xxv + 1,934 pp., DM 496 ($124.00).

Vol. III: Astronomie und Geophysik, 1952, xviii + 795 pp., DM 248 ($62.00).

Vol. IV: Technik

Part 1, Stoffwerte und mechanisches Verhalten von Nichtmetallen, 1955, xvi + 881 pp., DM 288 ($72.00).
Part 2, Stoffwerte und Verhalten von metallischen Werkstoffen.
2a, Grundlagen, Prüfverfahren, Eisenwerkstoffe, 1963, xii + 888 pp., DM 468 ($117.00).
2b, Sinterwerkstoffe, Schwermetalle (ohne Sonderwerkstoffe), 1964, xx + 1,000 pp., DM 530 ($132.50).
2c, Leichtmetalle, Sonderwerkstoffe, Halbleiter, Korrosion, 1965, xx + 976 pp., DM 518 ($129.50).
Part 3, Elektrotechnik, Lichttechnik, Röntgentechnik, 1957, xv + 1,076 pp., DM 396 ($99.00).

Volumes in Preparation

Vol. II: Eigenschaften der Materie in Ihren Aggregatzuständen

Part 1, Mechanisch-thermische Zustandgrössen.
Part 5, Physikalische und chemische Kinetik.
Part 10, Magnetische Eigenschaften II.

Vol. IV: Technik

Part 4, Wärmetechnik.

Landolt-Börnstein: Zahlenwerte und Functionen aus Naturwissenschaften und Technik, Neue Serie—Numerical Data and Functional Relationships in Science and Technology, New Series, K. H. Hellwege, editor-in-chief.

Volumes Published

Group I: Kernphysik und Kerntechnik - Nuclear Physics and Technology

Vol. I, Energy Levels of Nuclei: A = 5 to A = 257, A. M. Hellwege and K. H. Hellwege, eds., 1961, xii + 813 pp., DM 212 ($53.00).

Group II: Atom und Molekularphysik—Atomic and Molecular Physics

Vol. I, Magnetische Eigenschaften Freier Radikale—Magnetic Properties

of Free Radicals, K. H. Hellwege and A. M. Hellwege, eds., 1965, x + 154 pp., DM 68 ($17.00).

Group VI: Astronomie, Astrophysik und Weltraum-Forschung—Astronomy, Astrophysics and Space Research

Vol. I, Astronomie und Astrophysik—Astronomy and Astrophysics, H. H. Voigt, ed., 1965, xxxix + 711 pp., DM 314 ($78.50).

Other groups planned and volumes expected to be published in 1966 or 1967:

Group I: Nuclear Physics and Technology

Hilfstabellen für α-, β-, γ- Spektroskopie—Auxiliary Tables for α-, β-, γ- Spectroscopy.

Ladungs-und Dichteverteilung im Kern—Charge and Density Distribution in the Nucleus.

Group II: Atomic and Molecular Physics

Vol. I, Lumineszenz organischer Molekeln—Luminescence of Organic Molecules.

Mikrowellenspektroskopie von Molekeln—Microwave Spectroscopy of Molecules.

Molekularakustik—Molecular Acoustics.

Vol. II, Magnetische Eigenschaften der Koordinations und metallorganischen Verbindungen der Übergangselemente—Magnetic Properties of Coordination and Organo-metallic Compounds of Transition Elements.

Group III: Crystal and Solid State Physics

Elastische, elastoopische, piezoelektrische und andere Eigenschaften von Einkristallen - Elastic, Elasto-optic, Piezoelectric and Other Properties of Single Crystals.

Group IV: Macroscopic and Technical Properties of Matter

Phosphoreszenz anorganischer Substanzen - Phosphorescence (Luminescence) of Inorganic Substances.

Group V: Geophysics and Space Research

Aeronomy; Cosmic Radiation.

Published by Springer-Verlag, Berlin, Heidelberg, and New York. Also available from Walter J. Johnson, Inc., 111 Fifth Ave., New York, N.Y. 10003, and Stechert-Hafner, Inc., 31 E. 10th St., New York, N.Y. 10003.

5.2. TABLES DE 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 (IUPAC) and the editorship of Ch. 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. Between 1936 and 1945, 40 installments of the Tables Annuelles appeared. Each contained one or more chapters on special topics, some covering data of the periods 1931-1934 or 1935-1936, some the whole period 1931-1936, and No. 40 only, 1931-1939. Later 8 of these were issued as Volume XI and 12 as Volume XII. In 1947 publication was resumed under the title "Tables de Constantes Sélectionées." To date, expert collaborators have compiled 14 numbered monographs in this new series. The present director is Madame S. Allard, 250 rue Saint Jacques, Paris V^{e}, France. Guidance is provided by an advisory committee composed of eminent scientists. Publication of the new series has been supported by governmental grants, by contributions from industrial concerns, and by profits from sales.

Substances

The subject matter of a given monograph, both as to substance and properties, is designed to meet a current demand of science or industry for specialized tables. Both organic and inorganic substances have been covered (see list of publications at end of this section).

Properties

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, the properties reported being those of greatest significance in the chosen fields.

Sources of Data

World literature.

Critical Appraisal

There is some selection of values, but the criticality varies from one monograph to another. The goal is to produce "useful" as well as critical values. Where doubt exists, attention is called to the uncertainty. The editorial staff avails itself of guidance from collaborating scientists.

Use of Nomenclature, Symbols, Units, and Physical Constants

As far as possible, IUPAC usage is adhered to. If no rules exist, well-known and able authorities are followed.

Currency

There has been no definite plan to bring the earlier tables of the current series up to date. However, some subjects, particularly those for which few if any other compilations exist, are treated somewhat as a series, for example, Optical Rotatory Power, for which five volumes have been issued.

Format

Volumes 1 - 5 of the tables were paper-covered, Volumes 6 and 7 were issued with both paper and hard covers, and those since Volume 8 have hard covers, 8 1/4" x 10 7/8". The data are presented in tables. Arrangement of material varies because different substances and properties are treated in each monograph. A bibliographic column in the tables guides the user to the pertinent literature reference in the general bibliography at the end of the monograph. General

indexes vary in type, some being indexed by name, others by formula, and some by author with references to the general bibliography. Although the tables are in French, the title page and, beginning with Volume 6, the preface, introduction, and other explanatory sections such as those for symbols and abbreviations are given in both French and English.

Publication and Distribution

Tables de Constantes Sélectionnées - Tables of Selected Constants

Vol. 1. Longueurs d'Onde d'Émissions X et des Discontinuités d'Absorption X—Wavelengths of Emission and Discontinuities in Absorption of X-Rays, Y. Cauchois and H. Hulubei, 1947, 199 pp. (out of print).

Vol. 2. Physique Nucléaire—Nuclear Physics, R. Grégoire, F. Joliot-Curie, and I. Joliot-Curie, 1948, 131 pp. (out of print).

Vol. 3. Pouvoir Rotatoire Magnétique (Effet Faraday)—Magnetic Rotatory Power (Faraday Effect); R. de Mallemann, Effet Magnéto-Optique de Kerr—Magneto-Optic Effect (Kerr), F. Suhner, 1951, 137 pp., 15 F, £1.10.0. ($4.50).

Vol. 4. Données Spectroscopiques Concernant les Molécules Diatomiques—Spectroscopic Data for Diatomic Molecules, B. Rosen, R. F. Barrow, A. D. Caunt, A. R. Downie, R. Herman, E. Huldt, A. MacKellar, E. Miescher, and K. Wieland, 1951, 361 pp., 48 F, £5.0.0. ($15.00).

Vol. 5. Atlas des Longueurs d'Onde Caractéristiques des Bandes d'Émission et d'Absorption des Molécules Diatomiques—Atlas of Characteristic Wavelengths for Emission and Absorption Bands of Diatomic Molecules (a continuation of Vol. 4 by the same authors), 1952, 389 pp., 56 F, £5.15.0 ($17.50).

Vol. 6. Pouvoir Rotatoire Naturel I-Steroïdes—Optical Rotatory Powers I-Steroids, J.-P. Mathieu and A. Petit, 1956, 507 pp. (out of print).

Vol. 7. Diamagnétisme et Paramagnétisme—Diamagnetism and Paramagnetism, G. Foëx; Relaxation Paramagnétique—Paramagnetic Relaxation, C. J. Gorter and L. J. Smits, 1957, 317 pp., 97 F, £9.15.9. ($29.00).

Vol. 8. Potentiels d'Oxydo-Réduction—Oxidation-Reduction Potentials, G. Charlot, D. Bézier, and J. Courtot, 1958, 41 pp., 21.60 F, £1.10.0 ($5.00).

Vol. 9. Pouvoir Rotatoire Naturel II-Triterpénoïdes—Optical Rotatory Power II-Triterpenoids, J.-P. Mathieu and G. Ourisson, 1958, 302 pp., 93.60F, £7.0.0. ($21.00).

Vol. 10. Pouvoir Rotatoire Naturel III-Amino-acides—Optical Rotatory Power III-Amino Acids, J.-P. Mathieu, J. Roche, and P. Desnuelle, 1959, 61 pp., 28 F, £2.0.0. ($6.50).

Vol. 11. Pouvoir Rotatoire Naturel IV-Alcaloïdes—Optical Rotatory Power IV-Alkaloids, J.-P. Mathieu and M. M. Janot, 1959, 211 pp., 110.40 F, £8.0.0. ($24.00).

Vol. 12. Semi-Conducteurs—Semi-Conductors, P. Aigrain and J. Balkanski, 1961, 78 pp., 27 F, £2.0.0. ($6.50).

Vol. 13. Rendements Radiolytiques—Radiolytic Yields, M. Haïssinsky and M. Magat, 1963, 230 pp., 114 F, £8.10.0. ($25.50).

Vol. 14. Pouvoir Rotatoire Naturel Ia-Stéroïdes—Optical Rotatory Power Ia-Steroids, J. Jacques, H. Kagan, G. Ourisson, and S. Allard, 1965, 1,046 pp., 258 F.

Vol. 15. Données Relatives aux Sesquiterpenoïdes—Data Relative to Sesquiterpenoids, G. Ourisson, S. Munavalli, and C. Éhret, 1966, 70 pp.

In Preparation

Metals of High Purity, 1967
Refractory Compounds

There have been several publishers for the present series. Volume 8 and later volumes have been published by Pergamon Press from whom the earlier volumes as well as the titles, availability, and prices of the 40 installments of Tables Annuelles, covering the period 1931-1936, may be obtained.

Published by Pergamon Press, 4 and 5 Fitzroy Square, London, W.1, England; 122 E. 55th St., New York, N.Y., U.S.; and 24 rue des Ecoles, Paris V^{e}, France.

5.3. INTERNATIONAL CRITICAL TABLES

Organization

The compilation of the International Critical Tables (ICT) of Numerical Data, Physics, Chemistry, and Technology was recommended at the organizational meeting of the International Union of Pure and Applied Chemistry in 1919. In 1923, the enterprise was given the patronage of the International Research Council (now the International Council of Scientific Unions). The National Research Council of the National Academy of Sciences accepted editorial and financial responsibility on behalf of the United States and with the cooperation of the American Chemical Society and the American Physical Society created a board of trustees and a board of editors. The Board of Trustees

initially raised $170,000 for the project from 244 firms and individuals and two foundations. Later, a few additional contributions were received.

The Board of Editors appointed corresponding editors in many different parts of the world. The corresponding editors, in turn, appointed advisory committees to assist in the work. On the basis of recommendations of the corresponding editors, cooperating experts were selected and given the responsibility for critically compiling data for some 300 sections of the tables. Under the vigorous leadership of the editor-in-chief, Edward W. Washburn, the seven volumes of the ICT were published between 1926 and 1930 and were followed by a comprehensive index in 1933. Unfortunately, the provisions made for periodic revision were quite inadequate. In view of the scientific advances made since their publication, a complete revision in one series of volumes is out of the question. The many publications of excellent numerical property values, described elsewhere in this survey, provide in limited areas a substitute for revisions of the corresponding parts of the ICT.

Substances

Elements and compounds, both organic and inorganic, are appropriately covered in six of the seven volumes. Volume II is concerned with a variety of natural and industrial materials of technological interest for which composition and properties cannot be well characterized.

Properties

Volume I gives units and values for international and various national systems of weights and measures; symbols, basic constants, conversion factors, and atomic weights; values for thermometric scales; physical properties of chemical substances; crystallographic and x-ray data; and astronomic and geodetic data. Volume II, as mentioned above, provides useful data on important natural and industrial materials. Volume III treats PVT (pressure, volume, temperature) relations and phase equilibrium data. Volume IV contains additional phase equilibrium data, cryoscopic data, osmotic pressure, and properties of surfaces. Volume V gives additional data for many of the substances discussed in Volume I and, in addition, thermodynamic quantities. Volume VI treats x-ray data, electrical and electronic data, and magnetism and acoustics. Volume VII treats refractivity, kinetics, absorption spectra of dyes, viscosity of pure liquids,

thermodynamic data including a large section on free energy (Gibbs energy), and optical rotation.

Critical Appraisal

The ICT was the first comprehensive compilation in which all values were carefully appraised. The editors accepted only "best values" that cooperating experts could derive from all the information available, with an indication where possible of their probable reliability. The books are in English, but in each volume the table of contents, the preface, introduction, and when included, some tables, discussions, and definitions are also given in French, German, and Italian. The arrangement in the ICT of all chemical substances and of all systems that may be represented by a formula is in accordance with a system called the "Standard Arrangement" in which each element is given a key-number. This system was based upon the long form of the Periodic Table and in a revised form is now known as the Standard Order of Arrangement of the Elements. References include only direct sources of values given and sources of similar data if no values are given. Text, equations, graphs, charts, and tables were limited editorially by considerations of space.

Use of Symbols, Units, and Physical Constants

At the time of publication, the ICT could be taken as the international authority on units, symbols, and constants.

Currency

The plan was to publish data obtained from as complete a survey as possible of world literature through 1923. There was no complete coverage of the literature beyond 1923 though later data are included in some sections. Since the tables were published between 1926 and 1930, some data were obsolete at the time of publication. Even today, because of its comprehensiveness and compactness, the ICT is still widely used.

5.3.

Format

The ICT is issued in 8 1/2" x 11 1/4" bound books. There are seven volumes of tables and an index volume cumulative for the entire set. The index is arranged alphabetically except that under the name of a chemical substance the properties are listed before the systems of which the substance is one of the components. Data for a given system are listed only once, but cross-references are given to systems of which the referenced item is a component but which alphabetically appear earlier in the index.

Publication and Distribution

International Critical Tables of Numerical Data, Physics, Chemistry and Technology, published for the National Academy of Sciences - National Research Council, by McGraw-Hill Book Co., 330 W. 42nd St., New York, N. Y. 10036.

Vol. I, 1926, xx + 415 pp.	Vol. II, 1927, xviii + 616 pp.
Vol. III, 1928, xiv + 444 pp.	Vol. IV, 1928, viii + 481 pp.
Vol. V, 1929, ix + 465 pp.	Vol. VI, 1929, x + 471 pp.
Vol. VII, 1930, ix + 507 pp.	Index, 1933, vii + 321 pp.

Seven volumes and Index, $250.00; Vols. I-VII and Index, each $35.00.

Appendix

REFERENCES FOR NOMENCLATURE, SYMBOLS, AND CONSTANTS

1. Nomenclature of Inorganic Chemistry, IUPAC 1957 Definitive Rules, French and English on facing pages, Butterworth and Co. (Publishers), Ltd., London (1959), 2nd printing, 1965, $3.00. In U.S., Butterworth, Inc., Washington, D.C. 20014.

   a. English version reprinted in J. Am. Chem. Soc., 82, 5,523-5,544 (1960), reprint available from Chemical Abstracts Service, Box 1378, Columbus, Ohio 43216, gratis; also from IUPAC Secretariat, Basle, Switzerland, Swiss F 3.20.

   b. Japanese translation, entitled Muki Kagaku Meimeiho (by K. Yamasaki, Professor of Chemistry, Nagoya University), available from Nankodo Publishing Co., 23, Harukicho 3-chome, Bunkyoku, Tokyo, 1961, 73 pp., ¥ 280.

   c. Swedish translation in Svensk Kem. Tidskr., 72, 448 (1960); also published by Tekniska Nomenclaturcentralen, P.O. Box 5073, Stockholm 5, Sweden, KR 7.

   d. German translation in Chem. Ber., 92, 7 (1959), XLVII - LXXXVI.

   e. Czechoslovakian translation in Chem. Listy, 57, 494 (1963).

f. Dutch translations in (1) Mededel. Vlaam. Chem. Ver., 24, 108-166 (1962), available from Vlaamse Chemische Vereniging, Maria-Louiza Square 49, Brussels 4, Belgium, Belgian F. 70; (2) Chem Weekblad, 59, 149-176 (1963), available from Koninklijke Nederlandse Chemische Vereniging, Burnierstraat 1, The Hague, the Netherlands, HF1.5.

g. Bulgarian translation may be obtained from Professor Dr. B. Kurtev, Bulgarian Academy of Science, 1, rue du 7-Novembre, Sofia, Bulgaria.

h. Portuguese translation published in Rev. Port. Quim., 7, 32 (1965).

i. Yugoslav translation in preparation.

j. Persian translation in preparation.

Extensions to these rules (in English) appear in Compt. Rend. Conf. Union Intern. Chim. Pure Appl., 22nd Conference, July 1963, pp. 207-211, and of the 23rd Conference, July 1965, pp. 183-187.

2. Nomenclature of Organic Chemistry, IUPAC 1957 Rules. Definitive rules for (i) Section A–Hydrocarbons, (ii) Section B–Fundamental Heterocyclic Systems, and (iii) Nomenclature of Steroids; and Tentative Rules for Nomenclature in the Vitamin B-12 field, 1st edition, 1958, 2nd edition, 1966. [Includes corrections to 1958 edition and a revised index but omits Tentative Rules for Nomenclature in the Vitamin B-12 Field], Butterworth and Co. (Publishers), Ltd., London. In U.S. Butterworth, Inc., 7300 Pearl St., Washington, D.C. 20014. $5.00.

a. English version of (i) and (ii) with comments, reprinted in J. Am. Chem. Soc., 82, 5,545-5,574 (1960), reprint available from Chemical Abstracts Service, Box 1378, Columbus, Ohio 43216, $1.00; also from IUPAC Secretariat, Basle, Switzerland, Swiss F. 4.30. An English reprint also appeared in the "Handbook for The Chemical Society (London) Authors," 1961, pp. 47-131.

b. French version of (i) and (ii) published in the Bull. Soc. Chim., France, 1, January 1957, available from Maison Masson & Cie, 120, boulevard St-Germain, Paris VI^{e}.

c. Spanish translation of (i), (ii), and (iii) available from Professor J. Pascual Vila; Facultad de Ciencias, Universidad de Barcelona, Barcelona, Spain.

d. Japanese translation, Yuki Kagaku Meimeiho, available from Nankodo Publ. Co., 23, Harukicho 3-chome, Bunkyoku, Tokyo, Japan, 120 pp.(1959), ¥ 350.

e. Czechoslovakian translation of (i) and (ii) published in Chem. Listy, 56, 15 and 152 (1962).

f. Bulgarian translation of (i) and (ii) may be obtained from Professor Dr. B. Kurtev, Bulgarian Academy of Science, 1, rue du 7-Novembre, Sofia, Bulgaria.

g. Italian translation of (i) and (ii), "Nomenclatura di Chimica Organica," available from Tipografia Editrice Italia, via del Corso 20-21, Rome, Italy.

3. Definitive Rules for the Nomenclature of Amino Acids, Steroids, Vitamins and Carotenoids, IUPAC Commission on the Nomenclature of Biological Chemistry, first printed in Chem. Eng. News, 30, 4,522-4,526 (1952); Biochem. J., 42, 1 (1948), 52, 1-2 (1952); J. Biol. Chem., 169, 237-245 (1947).

   a. Reprinted in J. Am. Chem. Soc., 82, 5,575-5,584, reprint available from Chemical Abstracts Service, Box 1378, Columbus, Ohio 43216, gratis; also from IUPAC Secretariat, Basle, Switzerland, Swiss F. 3.20.

   b. Czechoslovakian translation in Chem. Listy, 57, 51, 151, 348, 350, 1963.

4. Nomenclature of Organic Chemistry, Definitive Rules, Section C–Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium and/or Tellurium, issued by IUPAC Commission on the Nomenclature of Organic Chemistry, Butterworth and Co. (Publishers), Ltd., London (1965). In U.S., Butterworth, Inc., Washington, D.C., $9.50. (Section C includes changes made in the 2nd edition of Sections A and B.)

5. Manual of Physico-Chemical Symbols and Terminology–Definitive, IUPAC, Physical Chemistry Section, Commission on Physico-Chemical Symbols and Terminology, 1959, French and English (facing pages), Butterworth and Co. (Publishers) Ltd., London (out of print).

   a. Reprinted in J. Am. Chem. Soc., 82, 5,517-5,522 (1960), includes annotation on American usage, available from Chemical Abstracts Service, Box 1378, Columbus, Ohio 43216, 50¢.

   b. Japanese translation published in Kagaku To Kogyo (Chemistry and Chemical Industry) in 1964.

   c. Russian translation published in Zh. Fiz. Khim. (Journal of Physical Chemistry), 34, 10, 2,381-2,389 (1960).

   d. Bulgarian translation may be obtained from Professor Dr. B. Kurtev, Bulgarian Academy of Science, 1, rue du 7-Novembre, Sofia, Bulgaria.

Note: Reprints of 1, 2, 3, and 5 from J. Am. Chem. Soc., 82, 5,517 (1960), paperbound together available under title "IUPAC Reports on Symbolism and Nomenclature" from Chemical Abstracts Service, $3.00. Pamphlets giving ACS Committee Reports on nomenclature of specific classes of compounds are also available from Chemical Abstracts Service (see their Catalog of Services, 1966).

6. Symbols, Units, and Nomenclature in Physics, IUPAP, SUN Commission, Document U.I.P. 11 (S.U.N. 65-3), - 1965, available from Professor

J. de Boer, Secretary, Instituut voor Theoretsche Fysica, Valckenierstraat 65, Amsterdam (C), the Netherlands. A reprint of the previous edition, Document U.I.P. 9 (S.U.N. 61-44)-1961, with comments on AIP usage by H. C. Wolfe, appeared in Phys. Today, 15, 6, 20-36, 1962.

7. International Organization for Standardization: ISO Recommendation R-31, Quantities, Units, Symbols, Conversion Factors and Conversion Tables. ISO Recommendation R-31 is issued in English, French, and Russian. Copies may be obtained through the respective national standards organizations; in the U.S., American Standards Association Inc., 10 E. 40th St., New York, N. Y. 10016.

   Part I: 1956, 1st edition, Fundamental Quantities and Units of the MKSA System and Units of Space and Time, $2.40.
   2nd edition, title changed to International System of Units and Quantities and Units of Space and Time (approved by ISO Council in 1965).

   Part II: 1958, 1st edition, Quantities and Units of Periodic and Related Phenomena, $1.80.

   Part III: 1960, 1st edition, Quantities and Units of Mechanics, $4.80.

   Part IV: 1960, 1st edition, Quantities and Units of Heat, $1.80.

   Part V: 1965, 1st edition, Quantities and Units of Electricity and Magnetism (approved by ISO Council in 1965).

   Part VII: 1965, 1st edition, Quantities and Units of Acoustics (approved by ISO Council in 1965).

   Part XI: 1961, 1st edition, Mathematical Signs and Symbols for Use in the Physical Sciences and Technology, $2.40.

8. Nomenclature for Terpene Hydrocarbons—Acyclics, Monocyclics, Bicyclics, Advances in Chemistry Series, 14, Am. Chem. Soc., 1955, Special Issue Sales Dept., American Chemical Society, 1155 Sixteenth St., N.W. Washington, D.C. 20036, $3.00.

9. The Naming and Indexing of Chemical Compounds, Chem. Abstr., 56, 1962, January-June, Subject Index, pp. 1N - 98N. Reprint, Chemical Abstracts Service, $5.00.

10. Glossary of Terms in Nuclear Science and Technology, prepared by the National Research Council, approved by the American Standards Association, and published by The American Society of Mechanical Engineers, New York, N.Y. 10016, $5.00.

11. New Values for the Physical Constants Recommended by NAS-NRC, Nat. Bur. Stand. U.S. Tech. News Bull., 47, 10, 175-177, 1963. Tables reprinted in Phys. Today, 17, 2, 48, 1964.

12. Values of the Fundamental Constants for Chemistry, IUPAC Commission on Thermodynamics and Thermochemistry and Commission on Physicochemical Data and Standards, F. D. Rossini, Pure Appl. Chem., 9, No. 3, 453-459, 1964. Reprint available from Butterworth and Co. (Publishers), Ltd., London, or Butterworth, Inc., Washington, D. C. 20014.

13. International Electrotechnical Commission: Letter Symbols to be Used in Electrical Technology, IEC Publication 27, 4th edition, French-English, 1966, $12.00. Available from American Standards Association, Inc., 10 E. 40th St., New York, N. Y. 10016.

14. International Electrotechnical Commission: Recommendations in the Field of Quantities and Units Used in Electricity, IEC Publication 164, French-English, 63 pp., $11.00. Available from American Standards Association, Inc., 10 E. 40th St., New York, N. Y. 10016.

Index

(Numerical code designations following index entry refer to section to which entry applies. Capital letters indicate title of project.)

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