

LINDA RAY ARMY

THE SEARCH FOR DATA

In the Physical and Chemical Sciences



THE SEARCH FOR DATA IN THE PHYSICAL AND CHEMICAL SCIENCES

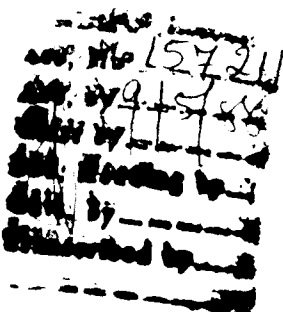
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PREFACE

The provision of numerical data in physics and chemistry is a fundamental part of my work in the Physical Sciences Library at the University of Massachusetts/Amherst. Often, these requests can be satisfied by using the standard handbooks kept at the desk or in the reference collection. But, for those requests that cannot be satisfied so easily, an inordinate amount of time and energy must be expended by either the librarian or the scientist to ferret out needed information. The difficulty of locating particular pieces of data among the many publications of the National Bureau of Standards first prompted me to consider access to data as a suitable topic for research. Thus, when the opportunity arose for me to take a sabbatical leave in the spring of 1982, I chose to use the time to study this problem.

The time and location independent data of physics and chemistry became the focus of my research. These data can be measured repeatedly and expressed numerically. (Spectral data and other data which are commonly presented graphically were excluded.) I set myself two goals: to investigate the nature, generation, collection, and retrieval of physical and chemical data in general, and to analyze and index National Bureau of Standards' compilations in particular. Writing this book has improved my understanding of the problems and techniques of data retrieval and increased my professional efficiency in reference work. I hope the accompanying "Guide to Selected NBS Data Compilations," contained in part 2 of this book, will be a useful tool to my colleagues.

The proliferation of acronyms in a book of this nature is unavoidable. I have attempted to include the acronym of an organization or other proper name when the name is introduced in each chapter, but this practice is at times awkward and distracting to the reader, particularly for those names in common use. Therefore, I have compiled a brief list of frequently used acronyms to which the reader can refer if the meaning of an acronym is not clear from its context:

CODATA:	Committee on Data for Science and Technology (of the International Council of Scientific Unions).
GPO:	U.S. Government Printing Office.
IUPAC:	International Union of Pure and Applied Chemistry.
JPCRD:	<i>Journal of Physical and Chemical Reference Data.</i>
NBS:	National Bureau of Standards.
NSRDS:	National Standard Reference Data System.
OSRD:	Office of Standard Reference Data.
SI:	Systeme International d'Unités (International System of Units, designated SI in all languages).

INTRODUCTION

In the third century B.C. Hieron II, king of Syracuse, is said to have had a crown made for him, purportedly of pure gold. But Hieron wished to know whether silver had not been added to the crown, debasing its value. He put the question to his adviser Archimedes, who was puzzled until one day, while at his bath, he realized that the volume of water displaced by a submerged object would equal the volume of the object itself and that by comparing the amount of water displaced by the crown to that displaced by an equal weight of gold, he could determine the presence of a lighter constituent metal. He was so pleased at his discovery that he ran home without his clothes, shouting, "Eureka, eureka!—I have found it, I have found it!"

What Archimedes had found was the principle of buoyancy, and in applying this principle to his problem, he had measured the density (that is, the mass per unit volume) of the crown and compared it to the density of an equal weight of pure gold, a standard sample. Thus, he both determined and used a specific datum: the numerical measurement of a physical property. The densities of gold and silver are now accurately established and widely used specimens of fundamental scientific data.

Throughout history, the progress of science has been dependent on the creation and use of physical property data. In the past, most data needs of the scientist could be met by a small number of journals and handbooks; judgments on the validity of data were often based on personal knowledge of the laboratory where the data were generated. Now, however, the enormous volume of the scientific literature and the greater number of scientists and laboratories performing measurements worldwide, combined with the complicated nature of modern research problems which are often cross-disciplinary, necessitate other means of obtaining needed data.

In recent times the data requirements of individual scientists have not been adequately met. In 1965, a survey of about sixteen thousand members of the American Chemical Society showed that, overwhelm-

ingly, current compilations of data satisfied poorly, or only moderately, the data queries of the respondents.¹ The value of current high quality data to industry is well-documented in the literature.²

In addition to the needs of pure research and industry, national policy decisions of profound importance are being made now which require massive amounts of accurate, quickly accessible data. The National Academy of Sciences specified those areas most affected: energy resources, environmental protection, space research, and defense. The academy estimated that a program adequate to evaluate and organize the data for these areas would cost less than one percent of the original cost of creating the data, but that to reach this level would require doubling or tripling current funding.³

The now popular and growing use of modelling and computer simulation to provide insight into modern scientific problems demands the availability of accurate data if it is to be of any value. An appropriate example is the study of ozone depletion in the atmosphere caused by the use of fluorocarbons. Estimation of the degree of depletion can only be calculated through the use of computer models of the atmosphere which require data from physics, chemistry, and meteorology. A model may be excellently conceived, but if the basic data then employed are wrong, the results will not correctly predict the behavior of the system simulated.

The origins of our current data requirements are thus threefold: the needs of basic research, the needs of industry, and the needs of government. The data exist, as we shall see, in great quantity. The difficulties lie in finding them when they are wanted and in determining their accuracy once they are found.

THE CREATION, COMPILATION, AND RETRIEVAL OF DATA

I

PART

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Temporem autem quinsud et aur

Chapter 1

The Nature of Data

The emphasis of this report is on the data of physics and chemistry—numerical measurements of specific physical and chemical properties of well-defined substances or systems. This restriction derives from a variety of reasons: (1) the interest of scientists in quantitative measurements in physics and chemistry, and the substantial contributions of this activity in advancing the progress of science; (2) the fact that most measurements of data in the natural sciences are founded on the principles of physics and chemistry; (3) the ability to control experimental conditions, which enables the measurement of physical and chemical properties to be repeatable, yielding consistently equivalent results that can be universally applied; (4) the need for physical and chemical data in all sciences; and (5) the original and continuing focus on physical and chemical data of such organizations as the National Bureau of Standards (NBS) and the International Council of Scientific Unions' Committee on Data for Science and Technology (CODATA).

The CODATA Task Group on Accessibility and Dissemination of Data has prepared an excellent analysis of the forms of data in its publication, "Study on the Problems of Accessibility and Dissemination of Data for Science and Technology."¹ The task group's definition of data is succinct: "A given piece of data generally refers to the magnitude of some *quantity* characterizing some *property or phenomenon* of a certain *system*, measured under a certain *condition*."² A simple example of a datum illustrating the four facets of this definition is the boiling point of ethyl alcohol. The system is, in this case, a chemical substance, C_2H_5OH . The property is the boiling point, the state at which the vapor pressure of the liquid is equal to the surrounding atmospheric pressure. The quantity is temperature. The measurement condition is standard atmospheric pressure.

Chapter 2

Locating Data in the Scientific Literature

From the vantage point of a data evaluation center, one can state . . . that the numerical data on materials properties in the world's primary literature is, in general, conflicting, confusing, and to a large degree inaccessible in a form which is useful to the end user. . . . Even the research sponsor and many other reviewers are not fully abreast of it. Therefore, the millions of dollars of research investment in public funds do not fully benefit the end user as intended. To the casual observer it almost seems that our past and current research funding policies are tailored to support nice people in universities and research laboratories to work on problems which excite them, simply to satisfy their curiosity. Research funds even provide support to enable the researcher to publish his findings and, thus, satisfy his ego vis-a-vis a handful of his peers. At that point, the transfer of information seems to stop, in a way daring the intended user to find it, understand it, decide on its validity and applicability, and use it if he dares. Few of the intended users have the time, training, disposition, or temperament to enter this jungle of so-called "original research literature" and attempt to decipher it.

Y. S. Toulikian, 1920–1981¹

Other than by making the needed measurements themselves, scientists use many of the same channels for obtaining data as for obtaining other scientific information. Exchanges with professional colleagues, though they may seem at the time the most efficient, are almost inevitably the least reliable. The information obtained may depend on the colleague's memory, or it may consist of the colleague's unpublished data that have not been subjected to the scrutiny of a referee. The traditional primary literature—journals and technical reports—may have more accurate data, but these data are seldom found easily. Scien-

Chapter 3

Critical Evaluation

Unfortunately the scientific literature contains many erroneous values. Few scientists or engineers seem to have given much thought to the magnitude of the problem, and some probably regard every numerical entry in a handbook as revealed truth. Yet anyone who has had to seek a particular number in the literature and searched out a dozen or more reports, only to end up with a set of widely discrepant values, comes to realize that a substantial intellectual effort and a considerable background in the field are needed to arrive at reliable figures.¹

A scientist's professional productivity would seriously suffer if he needed to retrieve each piece of data from the literature himself. In addition to the growth of the volume of literature, there has been a proliferation of data produced by new instrumentation and through automated measurement processes. More work is interdisciplinary, necessitating the use of data produced in fields other than the scientist's own. Some assurance of the quality of data is vital. The need for control over this large quantity of data—to retrieve data scattered throughout the literature and to verify their accuracy—has led to the development of the data analysis or data evaluation center.

Data centers, staffed by scientists who are experts in their disciplines, are designed to collect data from the published literature (though sometimes data are also measured on site); to use careful, systematized techniques to assess their accuracy; and to compile the results into convenient, clear tables with appropriate documentation. This process is known as critical evaluation; the values published, critically evaluated data.

How is data evaluated? Usually, the first step is to reduce separate sets of data for the same property to the same units, temperature scale, and relation to relevant fundamental constants.² This is not often simple, especially when subsidiary data are considered. The author's experi-

Chapter 4

Data Centers

Data centers, also referred to as data analysis centers or data compilation centers, vary in size and in renown; each specializes in a specific technical area. Some are associated with programs such as the National Standard Reference Data System; some are independent but may do work for government agencies on contract. The National Bureau of Standards (NBS) operates centers at its own facilities. The data evaluation work of data centers has been described in general in the preceding chapter. Descriptions of representative data centers are collected in this chapter to illustrate their structure, functions, activities, and publications.

One of the most outstanding, vigorous, and respected data centers is the Thermophysical Properties Research Center (TPRC) at Purdue University. Founded by Yeram S. Touloukian in 1957, it was one of the first external data centers to be selected by the NBS in 1964 as a component of the National Standard Reference Data System. It was combined with three smaller centers in 1974 to form the Center for Information and Numerical Data Analysis and Synthesis (CINDAS) under the directorship of Touloukian, although each center retained its separate identity.¹

CINDAS is an internationally recognized center for the analysis of thermophysical and electronics property data. Its compilations are subject to the most rigorous technical review. Touloukian was a leader in developing the concept of critically evaluated data and an untiring advocate for the establishment of centers applying its principles in all fields.

The TPRC maintains thermophysical and thermochemical data on over sixty thousand compounds. An affiliated laboratory of CINDAS, the Properties Research Laboratory, measures thermal, electrical, and optical properties of materials over a wide range of temperatures.²

Chapter 5

A Brief History of Data Compilations

Early attempts at data compilations were usually individual efforts, with those by the famous German scientists, Beilstein, Gmelin, and Landolt and Börnstein among the first. They were primarily descriptive, with data extracted from the literature and subjected to only minimal evaluation.¹ Later, in England, Kaye and Laby produced their *Tables of Physical and Chemical Constants*. In France, the *Tables Annuelles de Constantes et Données Numeriques* was published in ten volumes from 1910–1930; this was also a collection of unevaluated data.

The first compilation subjected to rigorous evaluation was the *International Critical Tables*, which took over ten years to complete. The tables were prepared in part at the request of the International Union of Pure and Applied Chemistry under American editorship and under the auspices of the International Research Council (a precursor to the International Council of Scientific Unions) and the National Academy of Sciences. The introduction states: "The word 'critical' [in the title] means that the cooperating expert was requested to give in each instance the 'best' value which he could derive from all the information available, together, where possible, with an indication of its probable reliability."² Many scientists were involved in this process, each, as stated, an expert in his specific subject area.

The *International Critical Tables* quickly became a standard reference work. As late as 1965, it was cited as the third most frequently consulted source by chemists for property data.³ Though its contents are dated, it is still widely used. Scientists throughout the world have always hoped that a revision or supplements to the *Tables* would be produced. However, in 1955, the National Research Council's Committee on Tables of Constants, which had taken much of the editorial and

Chapter 6

Selection Sources for Handbooks and Data Compilations

The standard tools of book selection serve to some extent to inform the librarian of newly published handbooks in physics and chemistry, and it is not necessary to discuss these here. Their coverage, however, is not always complete or as timely as might be desired. Consequently, it is appropriate to review here other sources that are specifically concerned with the publications of handbooks and data compilations. Many of these sources already have been discussed; the reader will be directed to the appropriate chapter for more information.

Two indexing services discussed in chapter 2 are useful sources of information about new handbooks. Current issues of *Physics Abstracts* list and abstract new data compilations or handbooks under the classified entry 01.30K: "Handbooks, dictionaries, tables and data compilation." (If a compilation's abstract is entered under a subject term rather than this general one, it will be cross-referenced here.) Both monographs and journal articles are cited. The semiannual subject index indexes these items under the entry "Collections of physical data." *Current Physics Index* uses the same classification but abstracts only monographic data compilations. However, it does also index here (01.30K) reviews of handbooks that have appeared in American Institute of Physics journals.

"Recent Data Compilations" is a section appearing in the last issue of each volume of the *Journal of Physical and Chemical Reference Data*. This lists new compilations, arranged by broad subject areas. It is not restricted to National Standard Reference Data System or National Bureau of Standards materials. Complete bibliographic informa-

Chapter 7

Data Journals and Related Publications

Experimental data are regularly reported in the journal literature, but there are journals whose main, or in some cases, sole purpose is the publication of experimental data. These are known as data journals. Some publish compilations, others report original results. Without doubt, the most valuable of these is the *Journal of Physical and Chemical Reference Data*. In this chapter are analyses both of important data journals and of continuously revised data compilations appearing in other research journals.

Atomic Data and Nuclear Data Tables, vol. 12– . New York: Academic Press, 1973– . Bimonthly.

Formed by the merger of *Atomic Data* and *Nuclear Data Tables*, this journal publishes compilations of experimental data and theoretical results of calculations in the subject areas indicated in the title. The data are timely but not always critically evaluated. Editorial policies require a standard format: a statement of the scope of the compilation; an historical review and analysis of scientific theory; a description of evaluation methods and treatment of errors; and a complete list of symbols. Partially cumulative author and subject indexes appear in even numbered volumes.

International Journal of Chemical Kinetics, vol. 1– . New York: Wiley Interscience, 1969– . Monthly.

This journal frequently publishes research in which new data are reported. Its scope is not restricted to articles of this sort, nor is it so rigorous as other titles in its requirements for the presentation of data or the provision of documentation on their generation. There are subject and compound indexes, the latter particularly useful for finding

Chapter 8

The National Bureau of Standards

The National Bureau of Standards (NBS) officially began operations on July 1, 1901, as a national laboratory devoted to measurements, units, and standards. The first director, Samuel S. Stratton, supervised a staff of ten: three physicists, a mechanic, two laboratory assistants, a clerk, a messenger, a watchman, and a laborer. Congress outlined the work of the National Bureau of Standards in its initial legislation. As used in the passage from the original legislation below, "standards" refer to units of measurement.

The functions of the bureau shall consist in the custody of the standards; the comparison of the standards used in scientific investigations, engineering, manufacturing, commerce, and educational institutions with the standards adopted or recognized by the government; the construction, when necessary, of standards, their multiples and subdivisions; the testing and calibration of standard measuring apparatus; the solution of problems which arise in connection with standards; the determination of physical constants and the properties of materials, when such data are of great importance to scientific or manufacturing interests and are not to be obtained of sufficient accuracy elsewhere.¹

In 1903, "National" was dropped from the name of the bureau when it was transferred from its original location in the Treasury to the Department of Commerce. So far as is known, the only reason for this change was that the new secretary preferred the name to resemble those of similar bureaus in Commerce such as the Coast and Geodetic Survey and the Geological Survey. In 1934, because of the proliferation of state and local "bureaus of standards" the qualifier "National" was restored.

Since its founding, the National Bureau of Standards has participated in basic research and technological or applied research.² This resulted

Chapter 9

The Retrieval of NBS Data Compilations

The National Bureau of Standards publishes several indexes and continuing bibliographies that enable the librarian or scientist to find older NBS publications and to learn of new ones. Unfortunately, their usefulness in locating data compilations is restricted by their very comprehensiveness. Because most of them cover all the output of the bureau, they necessarily cannot or, in any event, do not provide the specific indexing required to make compilations quickly accessible. There are two sources more limited in size and more detailed in indexing that cover only National Standard Reference Data System (NSRDS) publications; these are treated in other chapters of this report. (See chapters 7 and 10.) However, as one covers only articles from the *Journal of Physical and Chemical Reference Data* and the other is not (as yet, at least) a serial, it is often necessary to consult the broader sources described here. One must always do so if the compilation is not an NSRDS one.

Below are descriptions of those sources that cover NBS publications in general and analyses of how they may be used to retrieve data compilations. Titles are presented in order of importance. (It is assumed the reader is aware of the *Monthly Catalog of United States Publications* and needs no introduction to it.)

Publications of the National Bureau of Standards, 1966/67- . National Bureau of Standards Publication 305 and 305 Supplement 1-
Washington: Government Printing Office, 1969- . Annual.

The Publications is currently compiled by the Technical Information and Publications Division of the National Bureau of Standards. The series continues earlier indexes, NBS Circular 460 and its supplement,

Chapter 10

The National Standard Reference Data System

The rapid increase in the quantity and diversity of scientific information prevented established data compilers, including the National Bureau of Standards, from maintaining even approximate currency in their work, and their efforts were insufficient to meet scientific and industrial needs. This situation, combined with the frequent appearance of conflicting and inconsistent data, highlighted the need for a system of evaluation of reported data that, once created, could be used with confidence. If administered on a national scale, such a system would also help reduce the duplication of compilations by individual scientists and institutions.

In 1963, the Federal Council for Science and Technology recommended to the Director of the President's Office of Science and Technology that the National Standard Reference Data System (NSRDS) be established within the National Bureau of Standards. The bureau was the logical location for the system, considering its long tradition of work in evaluation and compilation of data.¹

The program was formally established by Public Law 90-396, the Standard Reference Data Act of 1968, which authorized the Secretary of the Department of Commerce "to provide or arrange for the collection, compilation, critical evaluation, publication, and dissemination of standard reference data."² As before, the NBS was charged with administration of the system, the establishment of associated Standard Reference Data Centers, and the coordination of similar work in other federal agencies.³

Data compilation work of the National Standard Reference Data System is concentrated on the "well-defined physical and chemical properties of substances and systems which are well-characterized,"

Chapter 11

Other National and International Programs

CODATA

The coordination of data collection and dissemination activities on an international scale is the responsibility of CODATA, the International Council of Scientific Unions' Committee on Data for Science and Technology. The nongovernmental International Council of Scientific Unions (ICSU) was founded in 1919 as the International Research Council, changing to its present name and structure in 1931. The membership is composed of various international scientific societies, such as the International Union of Pure and Applied Physics, the International Union of Pure and Applied Chemistry, the International Astronomical Union, and the International Union of Geodesy and Geophysics. Over sixty countries are represented in the various member unions. Partially funded by UNESCO, the ICSU holds annual general assemblies of its member unions and supports and instructs the work of its committees, such as the Committee of Space Research and the Committee on Science and Technology in Developing Countries.

The Committee on Data for Science and Technology of the International Council of Scientific Unions was formed in 1966. Its purpose, as stated in its constitution, is "to promote the evaluation, and in general the quality control of data and the methods by which they are acquired."¹ CODATA does not aim to publish large data compilations itself, but to encourage the production and distribution of critically evaluated data in the sciences and technology; to learn of centers engaged in such work and monitor, advertise, and coordinate their activities with other data centers; to alert scientists of the need to promote data programs in their own countries; to standardize methods of data handling and presentation; and to provide key values in thermodynamics and fundamental physical constants.² Originally, CODATA was con-

Chapter 12

Online Access to Data

Most academic reference librarians are accustomed to accessing bibliographic databases online. Such practices have increased librarians' efficiency and enabled them to offer new services. Nonbibliographic databases are far less familiar. Of these, directory, statistics, or business files are the most common. Property databases form the smallest group available from major vendors. As late as 1979, only 9 out of 230 total files accessible to institutions other than the sponsoring organizations contained physical or chemical data.¹

Property data systems are usually designed only to meet local needs, providing features considered valuable to the research laboratory or company served. This individualized, independent development has given rise to many problems, the most critical among them the lack of standardization not only for software but for query languages, which greatly inhibits data exchange or intersystem communication. One possible solution—not as yet financially worthwhile—would be to have a commercial vendor create interface software that would translate commands of the end user into the appropriate commands devised for a particular file. Until some solution is developed, it is probable that only laboratories and special libraries will be able to use most property data systems.

Other problems innate to property data systems will delay the expansion of their use. Locally developed systems usually contain only a few substances or properties, whereas, according to the Chemical Abstracts Service, about eleven hundred terms are required to designate most of the known physical and chemical properties.² Documentation for systems seldom records what, if any, evaluation has been applied to the data; sometimes error estimates are not included. Performing a search often requires learning a complicated query language. Software has been slow to develop for a user-oriented, interactive mode. Collection,

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PART

DATA COMPILATIONS
OF THE
NATIONAL BUREAU
OF STANDARDS

Energetics of Gaseous Ions

Microwave Spectral Tables

JANAS Thermochemical Tables

Selected Properties of Hydroge

Me V Total Neutron Cross Sectio

Transition Nettle Oxides: Crystal Chen

Introduction

Librarian: Yes ma'am, may I help you?

Scientist: Quick, young man! I need Doppfeldinger's coefficient for gases.

Librarian: Right away, ma'am. Er, what *is* Doppfeldinger's coefficient?

Scientist: Well I'm not exactly sure, really, but Dr. Winthrop down the hall told me I could use it to calculate the intermolecular pair potential of my system using this equation. [Shows librarian equation given below, which he undoubtedly finds *most* helpful:]

$$\phi(r\theta_1\theta_2\phi) = \phi_s r + \phi_{ns}(r\theta_1\theta_2\phi)$$

I'm in organic, you know, and it's not my field.

Librarian: (with wan smile) Ah, yes, well, what is this equation used for?

Scientist: For determining equilibrium and transport properties.

Librarian: Transport properties?

Scientist: You know, heat and mass transfer. I need to find the rate of diffusion.

Librarian: (with marked relief) Oh, chem engineering!

Scientist: (thinking to herself) Well, what did he think I was talking about. I could have told him that in the first place.

Librarian: (thinking to himself) Why didn't she tell me so in the first place!

Librarian: Let's try Lange's . . . H'mm, no listing for Doppfeldinger's coefficient here. Let me try Perry's. Ah, yes, here we are, Doppfeldinger's coefficient at 25°C. (Whew!)

Scientist: But I need it for high temperatures.

Librarian: I see; uh, did you try the *Handbook of Chemistry and Physics*?

Scientist: (growing impatient) Of course I did—before I ever even came in here.

Librarian: Well, let's try the subject catalog. . . . But wait, it seems to me I recall an NBS publication on diffusion coefficients—might that be related?

Scientist: Perhaps; yes, I think so—let's look at it. How can we find it?

Librarian: Uh, oh.

Is there an academic reference librarian in a general science library who has not experienced a similar situation?

A researcher approaches the desk, needing a particular piece of data—the numerical measurement of a physical property of a specific substance. The standard handbooks have not helped him: either the right substance is not listed or the range of experimental parameters is insufficient. To complicate matters, the scientist may be using a term unfamiliar to the librarian, and a master's degree in chemistry won't provide one with facility in the vocabulary of high energy physics. Explaining the context of the term so that the librarian can know whether to try thermodynamics handbooks or solid state sources may prove time consuming and difficult, particularly if the scientist is seeking data obtained in a field other than his own and has himself only a vague idea of its nature.

At this point the librarian may imperfectly recall the existence of the sort of table wanted in one of the many compilations of the National Bureau of Standards—but which one? He hesitates to tackle the *Publications of the NBS* because of its cumbersome arrangement, arcane keyword index of inconsistently chosen entry terms, and inclusive coverage of the entire published output of the NBS, of which data publications form only a tiny percentage. But how otherwise can it be found? Most academic libraries do not catalog numbers of NBS series individually. Annoyance glitters in the eyes of the inquirer and the librarian begins to despair.

It is with the hope of alleviating this difficulty that I have here reviewed, analyzed, and indexed those NBS publications that contain substantial compilations of high quality data. The most important aspects of the data in each have all been determined: the substance investigated, the properties measured, the experimental conditions, and the degree to which critical evaluation has been applied. Bibliographic relationships with other publications are traced. The index is designed for the retrieval of data by one not necessarily an expert in all aspects of physics and chemistry.

The compilation of this analysis has improved my own understanding of the various NBS series and of the structure and purpose of the National Standard Reference Data System. I hope it may also render NBS-gathered data more accessible to others.

Chapter 13

NBS Series Concerned with Data Compilations

National Bureau of Standards (NBS) data compilations are published for the agency by the Government Printing Office (GPO), the National Technical Information Service (NTIS), and selected commercial publishers. Most are now funded, at least in part, by the Office of Standard Reference Data (OSRD) of the National Standard Reference Data System (NSRDS). Access to NBS data compilations using the sources provided by the NBS has been discussed in part 1, chapters 9 and 10.

For most academic librarians, only those series published by the GPO and received as depository items are readily available. Consequently, only those series, with one exception, the *Journal of Physical and Chemical Reference Data Supplements*, are included here in part 2.

The NBS prints on the inside front covers of each of its publications an annotated list of its current series. A copy is reproduced here as Figure 3, "NBS Technical Publications." Because the descriptions provided by the bureau are sometimes vague, supplemental descriptions of those series likely to contain data compilations or related material are given below. The specific pertinence of a series to data compilation or evaluation work is reviewed, and the inclusion of certain numbers in this review is justified when necessary. Unless otherwise indicated, quotations are from the NBS annotations. Abbreviations given after the series title are those used by the NBS. Information is also provided for superseded series and the *JPCRD* supplements.

Circulars

NBS Circulars were published from 1903 to 1959. The series has been superseded by the monographs. Unless a circular bears some biblio-

Chapter 14

Guide to Selected NBS Data Compilations

In this section, individual data compilations prepared by the National Bureau of Standards (not just NSRDS-funded work) are analyzed and indexed. To be included, a compilation must contain tabulated property data for more than just a few substances and be of use to a physicist, chemist, or researcher in a closely related discipline; data used solely for applications purposes are not included. Critical reviews are also excluded. Graphically presented data for which corresponding numerical values are not provided are excluded or less thoroughly analyzed; this guide is intended to direct the user to readily available numerical quantities.

Bibliographic entries are arranged by NBS series title. Author, title, and date of publication comprise the entry; the GPO is the publisher of all the entries listed except for the *Journal of Physical and Chemical Data Supplements*. The following information is included after the entry:

1. The bibliographic relationship of the given title to other publications. If a publication has been updated in the *Journal of Physical and Chemical Reference Data (JPCRD)*, this is stated.
2. Whether the data have been critically evaluated, though this is not always feasible for older titles published before the concept of critical evaluation was developed. For all such entries, some indication of the quality of the data and whether they were experimentally determined or calculated is given.
3. The arrangement of information and tables.
4. The substance or system under investigation.

INDEX TO SELECTED NBS DATA COMPILATIONS

This index is arranged alphabetically by property. Each main entry has been chosen from the form appearing most commonly in the literature. The property subheadings that follow are presented as they appear in the publication indexed. (Terminology varies among the original publications, and this device has been employed in an attempt to collect like properties.) Copious cross-references have been provided to aid the user unfamiliar with the subject areas covered and to supply, it is hoped, some avenue to the correct term no matter how it is asked for. The occurrence of a cross-reference to another term should not be taken to mean that the two terms are equivalent. Indeed, the first may not even be a property but only a related concept to which someone might refer when asking about data. Main entries are also not entirely restricted to properties; in a very few cases, other types of information (e.g., "spectroscopic notation") have been entered in the index if they form a significant or useful accessory part of a compilation. Some properties given in the guide that are not uniquely distinguished by their names alone (for example, "statistical weights") are not indexed nor even given as cross-references when it can reasonably be expected that other indexed terms will be used in describing the needed information.

Following the property subheading, the symbol or symbols used in the original publication are provided to help the user ascertain whether the quantity is in fact that which he is seeking. The next column gives a brief indication of the substance or system under investigation. (If two property subheadings are exactly the same, entries are subarranged alphabetically by the substance or system.) Check the bibliographic entry for a more complete account of the nature of the system.

The last column contains an abbreviated notation for the publication indexed. A list of abbreviations is given below. After finding an appro-

APPENDIX A

National Standard Reference Data System

The National Standard Reference Data System comprises the set of data centers and other data evaluation projects administered or coordinated by the National Bureau of Standards. The primary aim of this program is to provide critically evaluated numerical data, in a convenient and accessible form, to the scientific and technical community of the United States. A second aim is to advance the level of experimental measurements by providing feedback on sources of error in various measurement techniques. Through both these means, the program strives to increase the effectiveness and productivity of research, development, and engineering design.

The technical scope of the program is restricted to well-defined physical and chemical properties of substances and systems which are well-characterized. While this definition leaves some borderline cases, the intent is to concentrate the effort on intrinsic properties which are clearly defined in terms of accepted physical theory. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. Likewise, materials of uncertain or variable composition are not included. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

In terms of the major applications of the outputs, current projects fall into the following categories:

Energy and Environmental Data—This program includes projects dealing with data that have an important application in some aspect of energy R&D or environmental quality improvement. Projects in chemical kinetics, nuclear properties, spectroscopic data, and interaction of radiation with matter are currently incorporated in this program. The output of these projects is particularly important in R&D on new energy sources, environmental monitoring techniques, and prediction of the effects of pollutants introduced into air, water, or land.

Industrial Process Data—Projects dealing with thermodynamic, transport, colloid and surface, and physical properties of industrially important substances are included in this program. Such data have particular application to design of new processes in the chemical and metallurgical industries, optimization of currently used processes, and general productivity enhancement.

Materials Utilization Data—This program covers properties required for material selection and R&D on new materials. The structural, optical, electric, magnetic and mechanical properties of solid materials are included.

Physical Science Data—Projects which involve basic data of very broad applicability, or which are associated with an important frontier field of science, are included in this program. Examples are fundamental physical constants, data on fundamental particles, and data relevant to radioastronomy.

The principal output of the program consists of compilations of evaluated data and critical reviews of the status of data in particular technical areas. Evaluation of data implies a careful examination, by an experienced specialist, of all published measurements of the quantity in question, leading to the selection of recommended value and a statement concerning its accuracy or reliability. The techniques of evaluation depend upon the data in question, but generally include an examination of the method of measurement and the characterization of the materials, a comparison with relevant data on other properties and materials, and a check for consistency with theoretical relationships. Adequate documentation is provided for the selections of recommended values and accuracy estimates.

The National Standard Reference Data System is managed by the Office of Standard Reference Data of the National Bureau of Standards. This office has the responsibility for allocating that part of the NBS budget which is spent on critical data evaluation, both within the NBS technical divisions and through contracts with outside organizations. The staff of the office act as monitors for all projects which are supported. The management of the publications program of NSRDS is also in the hands of OSRD, and an information service is operated on a limited scale. In addition, OSRD maintains close contact with other data compilation activities, both in the United States and abroad. It attempts, both domestically and internationally, to avoid needless duplication and to encourage coverage of important technical areas.

Evaluated data produced under the NSRDS program are disseminated through the following mechanisms:

Journal of Physical and Chemical Reference Data—A quarterly journal containing data compilations and critical data reviews, published for the National Bureau of Standards by the American Institute of Physics and the American Chemical Society.

NSRDS-NBS Series—A publication series distributed by the Superintendent of Documents, U.S. Government Printing Office.

Appropriate publications of technical societies and commercial publishers.

On-line retrieval systems, such as the NIH/EPA Chemical Information System (CIS) and other computer-readable formats.

Response by OSRD and individual data centers to inquiries for specific data.

Further information on NSRDS publications, sources of data, and support of data compilation activities can be obtained from:

Ms. Cynthia A. Goldman
National Bureau of Standards
Office of Standard Reference Data
Physics Building, Room A-320
Washington, D.C. 20234
Telephone: (301) 921-2228

NSRDS DATA CENTERS

Alloy Data Center

Dr. L. H. Bennett
Center for Materials Science
Materials Bldg.—Room B150
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2982

Aqueous Electrolyte Data Center

Dr. B. R. Staples
Center for Thermodynamics and
Molecular Science
Chemistry Bldg.—Room A164
National Bureau of Standards
Washington, D.C. 20234
(301) 921-3632

Atomic Collision Cross Section Information Center

Dr. E. G. Beaty
Joint Institute for Laboratory Astrophysics
University of Colorado
Boulder, Colorado 80309
(303) 492-7801

Atomic Energy Levels Data Center

Dr. W. C. Martin
Center for Radiation Research
Physics Bldg.—Room A167
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2011

Atomic Transition Probabilities and Atomic Line Shapes and Shifts Data Center

Dr. W. L. Wiese
Center for Radiation Research
Physics Bldg.—Room A267
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2071

Center for Information and Numerical Data Analysis and Synthesis (CINDAS)

Dr. Y. S. Touloukian
Purdue University
CINDAS
2595 Yeager Road
West Lafayette, Indiana 47906

(317) 463-1581/(800) 428-7675
Direct inquiries to: Mr. W. H.
Shafer

**Chemical Kinetics Information
Center**

Dr. R. F. Hampson, Jr.
Center for Thermodynamics and
Molecular Science
Chemistry Bldg.—Room A166
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2565

**Chemical Thermodynamics Data
Center**

Mr. D. D. Wagman
Center for Thermodynamics and
Molecular Science
Chemistry Bldg.—Room A152
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2273

Cryogenic Data Center

Mr. N. A. Olien
Center for Mechanical Engineer-
ing and Process Technology
National Bureau of Standards
Boulder, Colorado 80303
(303) 499-1000/Ext. 3257

Crystal Data Center

Dr. A. D. Mighell
Center for Materials Science
Materials Bldg.—Room A221
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2950

Diffusion in Metals Data Center

Dr. D. B. Butrymowicz
Center for Materials Science
Materials Bldg.—Room A153
National Bureau of Standards
Washington, D.C. 20234
(301) 921-3351

**Fundamental Constants Data
Center**

Dr. Barry N. Taylor
Center for Absolute Physical
Quantities
Metrology Bldg.—Room B258
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2701

***Fundamental Particle Data Cen-
ter**

Dr. Robert Kelly
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720
(415) 486-5885

***High Pressure Data Center**

Dr. Leo Merrill
5093 Harold B. Lee Library
Brigham Young University
Provo, Utah 84601
(801) 374-1211/Ext. 4442

Ion Energetics Data Center

Dr. Sharon Lias
Center for Thermodynamics and
Molecular Science
Chemistry Bldg.—Room A139
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2793

***Isotopes Project**

Dr. Janis Dairiki
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720
(415) 486-6152

Molecular Spectra Data Center

Dr. F. J. Lovas
Center for Thermodynamics and
Molecular Science
Physics Bldg.—Room B268

National Bureau of Standards
Washington, D.C. 20234
(301) 921-2021

Molten Salts Data Center
Dr. G. J. Janz
Rensselaer Polytechnic Institute
Department of Chemistry
Troy, New York 12181
(518) 270-6344

**Phase Diagrams for Ceramists
Data Center**
Dr. Lawrence P. Cook
Center for Materials Science
Materials Bldg.—Room A227
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2844

Photonuclear Data Center
Dr. E. G. Fuller
Center for Radiation Research
Radiation Physics Bldg.—Room
B109
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2625

Radiation Chemistry Data Center
Dr. Alberta B. Ross
University of Notre Dame

Radiation Laboratory
Notre Dame, Indiana 46556
(219) 283-6527

***Superconductive Materials Data
Center**
Dr. B. W. Roberts
General Electric Company
Research & Development Center
P.O. Box 8
Schenectady, New York 12301
(518) 585-8501

**Thermodynamics Research Cen-
ter**
Dr. Kenneth R. Hall
Texas A & M University
Department of Chemistry
College Station, Texas 77843
(713) 846-8765 or 845-4971

**X-Ray and Ionizing Radiation
Data Center**
Mr. J. H. Hubbell
Center for Radiation Research
Radiation Physics Bldg.—Room
C313
National Bureau of Standards
Washington, D.C. 20234
(301) 921-2685

*The Office of Standard Reference Data is not involved at the present time in the administration or funding of these data centers, but it does assist in making their outputs and services known to the scientific community.

†Since 1981, Dr. C. Y Ho has been director of CINDAS.

APPENDIX B

Standard Reference Data National Measurement Laboratory

Introduction

Reliable information on properties of materials is required for a wide range of applications in industry, government, and academia. For example, physical and chemical properties play a key role in the design of industrial processes, the identification of potentially toxic substances in the environment, and the improvement of materials durability.

To provide the scientific and engineering community with reliable sources of data, the Office of Standard Reference Data (OSRD) at the National Bureau of Standards (NBS) develops data bases of evaluated physical and chemical properties of substances. The evaluations are carried out through a network of data centers and other projects which comprise the National Standard Reference Data System (NSRDS). Experienced researchers in these centers assess the accuracy of the data reported in the literature, prepare compilations, and recommend the best values. The data bases are then made available through publications, magnetic tapes, and on-line systems.

The NSRDS was established in 1963 when the Federal Council for Science and Technology asked NBS to assume primary responsibility in the Federal Government for promoting and coordinating the evaluation of numerical data in the physical sciences. In 1968, Congress passed the Standard Reference Data Act, Public Law 90-396, providing a specific legislative mandate for the program. OSRD collaborates extensively with other Federal agencies and private sector organizations in carrying out this program.

Energy

A number of data compilations of interest to scientists and engineers working in such energy-related areas as nuclear technology, magnetic fusion, fossil fuel combustion, and energy storage have been assembled.

Data on the properties of rock salt were compiled to help in the design of nuclear waste isolation facilities. Evaluated rate constants for chemical reactions important in hydrocarbon combustion provide a basis for the design of more efficient fossil fuel systems.

A series of compilations on energy levels of highly ionized atoms gives important information for understanding magnetic fusion plasmas. Another series provides data on the properties of materials used in energy storage devices, including molten salts, flywheel materials (metals, alloys, nonmetallic composites), and metal hydrides.

Environment and Health

To develop procedures for assuring a clean environment, researchers must understand the interaction of pollutants with other materials in the biosphere. Through the Standard Reference Data program, data bases have been produced for identifying pollutants and modeling their effects on the environment. For example, a collection of over 33,000 mass spectra designed for detection and identification of pollutants is disseminated in published form, on magnetic tape, and through the Chemical Information System, an on-line computer network operated by the U.S. Environmental Protection Agency, National Institutes of Health, NBS, and other Federal agencies. Chemical kinetic data for modeling pollutant reactions, which determine the fate of undesirable substances in the atmosphere, are published regularly.

In the health-related area, a pilot project is underway to develop a radiation depth-dose data base for medical facilities that use linear accelerators in cancer treatment.

Industrial Design

Computer models are increasingly used to design and optimize industrial processes. However, to give valid answers, such models must be provided with reliable input data. Data bases of evaluated thermochemical and thermophysical properties, pertinent to a wide variety of industrial applications, are provided by the Standard Reference Data program. Comprehensive data bases are used by industry to determine the best and most energy-efficient method for producing a given chemical product. The regularly updated, loose-leaf publication, *Liquefied Natural Gas Materials and Fluids* handbook, supplies properties of materials important to the storage and transfer of liquefied natural gas. A new mathematical formulation for the properties of steam provides a complete description of its thermodynamic properties over the wide temperature and pressure ranges encountered in modern industrial uses. New program efforts will be directed toward developing techniques for predicting the properties of fluid mixtures.

Materials

To help improve the performance and durability of materials, the Standard Reference Data program provides data compilations that can be used to characterize corrosion processes, identify wear debris, and predict the diffusion of undesirable substances into structural materials.

Data on the structure of over 50,000 crystalline materials are provided in both printed and computer-based formats. A computer file of alloy phase diagrams is now being developed. A series of compilations on the diffusion of elements into copper and its alloys is widely used throughout industry. Also available are phase diagrams of ceramic materials and a comprehensive review on diffusion of organic substances into plastics such as polyethylene.

Information

The data bases produced by the Standard Reference Data program can be purchased in printed form; certain data bases are also available on magnetic tape and through on-line computer networks. The data bases are published by NBS, commercial publishers, and various technical and professional societies.

In cooperation with the American Chemical Society and the American Institute of Physics, OSRD publishes the quarterly *Journal of Physical and Chemical Reference Data*. Searches for specialized information are available through the program's technical information service.

For further information on the NBS Standard Reference Data program, write to or call:

Office of Standard Reference Data
A320 Physics Building
National Bureau of Standards
Washington, DC 20234
301/921-2228

NSRDS Data Centers

The following data centers, unless otherwise indicated, are located at the National Bureau of Standards, Washington, DC 20234:

Alloy Data Center
B150 Materials Building
Aqueous Electrolyte Data Center
A164 Chemistry Building
Atomic Collision Cross Section Information Center
Joint Institute for Laboratory Astrophysics

University of Colorado
Boulder, CO 80309
Atomic Energy Levels Data Center
A167 Physics Building
Atomic Transition Probabilities and Atomic Line Shapes and Shifts Data Center
A267 Physics Building

Chemical Kinetics Information
Center
A166 Chemistry Building
Chemical Thermodynamics
Data Center
A152 Chemistry Building
Center for Information and Numerical
Data Analysis and
Synthesis
Purdue University
2595 Yeager Road
West Lafayette, IN 47906
Crystal Data Center
A221 Materials Building
Diffusion in Metals Data Center
A153 Materials Building
Fluid Mixtures Data Center
National Bureau of Standards
Boulder, CO 80303
Fundamental Constants Data
Center
B258 Metrology Building
Ion Energetics Data Center
A139 Chemistry Building
Molecular Spectra Data Center
B268 Physics Building

Molten Salts Data Center
Rensselaer Polytechnic Institute
Department of Chemistry
Troy, NY 12181
Phase Diagrams for Ceramists
Data Center
A227 Materials Building
Photonuclear Data Center
B109 Radiation Physics Building
Radiation Chemistry Data Center
University of Notre Dame
Radiation Laboratory
Notre Dame, IN 46556
Thermodynamics Research
Center
Texas A & M University
Department of Chemistry
College Station, TX 77843
X-ray and Ionizing Radiation
Data Center
C313 Radiation Physics Building

NOTES

Introduction

¹Herman M. Weisman, "Needs of American Chemical Society Members for Property Data," *Journal of Chemical Documentation* 7 (February 1967): 9–14. The results of this survey also showed that the most frequently sought properties were boiling point, melting point, solubility, and thermodynamic properties. (Any science reference librarian could have so informed the author.) The survey was used in advising the newly created National Standard Reference Data System of chemists' data needs.

²Cited below are sources that discuss the value of high quality data to industry:

A. A. Bondi, "On the Economics and Timing of Data Evaluation and Estimation in an Industrial Setting," *Journal of the American Society for Information Science* 30 (November 1979): 360–363. Adapted from the author's Alpha Chi Sigma award address, this article cites two reasons for the need for new data: (1) the discovery of new compounds or novel uses for old compounds; and (2) the development of processes operating under different pressure, temperature, or chemical conditions from those for which a property has previously been measured.

National Physical Laboratory, *Chemical Thermodynamic Data on Fluids and Fluid Mixtures: Their Estimation, Correlation, and Use; Proceedings of the NPL Conference, 11–12 September, 1978* (Guildford, Surrey: IPC Science and Technology Press, 1979). The first three papers of these proceedings document data needs in chemical engineering: "Industrial Uses of Thermodynamic Data" (R. M. Gibbons et al., pp. 8–24), "The Needs of Industry for Fluid Property Data for Heat Exchanger Design" (L. B. Cousins and D. Butterworth, pp. 25–34), and "Some Industrial Needs for Data on Fluid Properties—How They Are Met" (P. Rathbone, A. L. Horvath, and R. W. Wheelhouse, pp. 35–45).

D. G. Elliot, et al., "Thermophysical Properties: Their Effect on Cryogenic Gas Processing," in *Phase Equilibria and Fluid Properties in the Chemical Industry*, ed. Truman S. Storvick and Stanley I. Sandler, ACS Symposium Series 60 (Washington: American Chemical Society, 1977), pp. 289–308. The authors discuss the types of data needed for process design and the economic effect of the availability of adequate data on design.

Howard G. Hipkin, "Thermodynamic Data Needs in the Synthetic Fuels Industry," in *Phase Equilibria and Fluid Properties in the Chemical Industry*,

ed. Truman S. Storvick and Stanley I. Sandler, ACS Symposium Series 60 (Washington: American Chemical Society, 1977), pp. 390–417. The specific requirements for synthetic fuels processing are determined by analysis of the existing technology.

M. G. O'Reilly and B. Edmonds, "Physical Property Data—Can You Afford It?" *Chemical Engineer* (London), no. 328 (January 1978), pp. 61–63. The authors describe a typical chemical engineering problem and how data are obtained to solve it.

K. W. Reynard, "EDSU—Fulfilling Industrial Needs for Data," in *Data for Science and Technology, Proceedings of the 7th International CODATA Conference, 1980*, ed. Phyllis Glaeser (Oxford: Pergamon Press, 1981), pp. 451–456. The results of failures of companies to obtain data are reviewed here, in addition to the services of the Engineering Sciences Data Unit in England.

M. Schoenberg, "Data Gaps in Respect to Organic Industrial Chemicals," in *Data for Science and Technology, Proceedings of the 7th International CODATA Conference, 1980*, ed. Phyllis Glaeser (Oxford: Pergamon Press, 1981), pp. 447–450.

American Society of Mechanical Engineers, *The Technological Importance of Accurate Thermophysical Property Information, Proceedings of a Session of the Winter Annual Meeting, December 6, 1979*, ed. Jan V. Sengers and Max Klein, National Bureau of Standards Special Publication 590 (Washington: U.S. Government Printing Office, 1980). The six papers collected here review the value of high quality data in physics and chemistry to mechanical engineering and industrial process design.

³Numerical Data Advisory Board, Committee on Data Needs, *National Needs for Critically Evaluated Physical and Chemical Data* (Washington: National Academy of Sciences—National Research Council, 1978).

Chapter 1

¹CODATA Task Group on Accessibility and Dissemination of Data, *Study on the Problems of Accessibility and Dissemination of Data for Science and Technology*, CODATA Bulletin, no. 16 (Paris: International Council of Scientific Unions, Committee on Data for Science and Technology, 1975).

²*Ibid.*, p. 15. Emphases are the Task Group's.

³*Ibid.*, pp. 2–5.

⁴These levels of refinement are taken from Randolph C. Wilhoit, "Thermodynamic Data Projects at TRC," in *A Review of AIChE's Design Institute for Physical Property Data (DIPPR) and Worldwide Affiliated Activities*, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), p. 71.

Chapter 2

¹Y. S. Touloukian, "The Impact of Physical Properties Research on Technological Advancement," keynote address in *Proceedings of the Seventh Symposium on Thermophysical Properties*, ed. Ared Cezairliyan (New York: American Society of Mechanical Engineers, 1977), p. 1.

²Robert E. Maizell, *How to Find Chemical Information* (New York: Wiley-Interscience, 1979), p. 202.

³Donald T. Hawkins, "Problems in Physical Property Data Retrieval," *Journal of Chemical Information and Computer Science* 20 (August 1980): 143-144.

⁴David R. Lide, "Critical Data for Critical Needs," *Science* 212 (19 June, 1981): 1343.

⁵Denis Grogan, *Science and Technology, an Introduction to the Literature*, 3d ed. (London: Clive Bingley; Hamden, Conn.: Linnet Books, 1976), p. 142.

⁶Grogan, p. 142. One field that has experienced rapid change and extraordinary real growth in its production of data (that is, not simply an inflation of the volume of publication) is high energy physics. Its burgeoning development is well illustrated in the history of the data compilations produced by the Particle Physics Data Group, a committee of physicists located primarily at the University of California at Berkeley. In 1957, they published a report, UCRL-8030: "Data for Elementary Particle Physics," which was accompanied by a wallet card, a card small enough to fit (folded) in a wallet, containing information on atomic and nuclear constants and atomic particles. By 1963, two wallet cards were needed to accommodate added information on hadrons; by 1964, three wallet cards were necessary. In 1967, the wallet cards proved too bulky and sheets of paper with small print were issued, called "wallet sheets." One of the physicists in the Group, Arthur Rosenfeld, recalled, "In Russia, where there are two words for 'sheet,' one for a small sheet of paper and one for a bed sheet, physicists (translating the title) chose the latter, suggesting perhaps that we had not sufficiently reduced the bulkiness problem." Arthur H. Rosenfeld, "The Particle Data Group: Growth and Operations—Eighteen Years of Particle Physics," *Annual Review of Nuclear Science*, 25 (1975): 572. In 1968, the wallet sheet was replaced by a data booklet. Later editions of this booklet are now taken from the first two sections (Tables of Particle Properties, and Miscellaneous Tables) of the biennially produced, "Review of Particle Properties." See chapter 7.

⁷John O'Connor, "Data Retrieval by Text Searching," *Journal of Chemical Information and Computer Sciences* 17 (August 1977): 181-186.

⁸G. W. A. Milne and S. R. Heller, "NIH/EPA Chemical Information System," *Journal of Chemical Information and Computer Sciences* 20 (November 1980): 210.

⁹General Subject Index. *Chemical Abstracts* 94 (1981): 651.

¹⁰General Subject Index, *Chemical Abstracts* 94 (1981): 1970.

¹¹F. A. Tate, "Techniques for the Retrieval of Chemical Information; Dreams vs. Nightmares," *Pure and Applied Chemistry* 49 (1977): 1899-1900.

¹²G. C. Carter, "Numerical Data Retrieval in the U.S. and Abroad," *Journal of Chemical Information and Computer Sciences* 20 (August 1980): 150.

¹³John W. Murdock, "Numerical Data Indexing," *Journal of Chemical Information and Computer Sciences* 20 (August 1980): 132.

¹⁴David R. Lide, "Quality Control of Data in the National Standard Reference Data System," in *Information Management in the 1980s, Proceedings of the ASIS Annual Meeting, 1977* (White Plains, New York: Knowledge Industry Publications, Inc., for the American Society of Information Science, 1977), Part II, card 5, frame D-3.

¹⁵R. W. Powell and Y. S. Touloukian, "Thermal Conductivities of the Elements," *Science* 181 (14 September 1973): 1004-1005.

¹⁶William H. Evans, "Effects of Errors in the Chemical Literature on the Compilation of Critically Evaluated Data," *Journal of Chemical Documentation* 6 (August 1966): 135-136.

¹⁷The list of questions is adapted from Maizell, *How to Find Chemical Information*, p. 208-210 and Carter, "Numerical Data Retrieval," p. 149.

¹⁸Maizell, p. 184.

¹⁹S. A. Rossmassler, "Presentation of Data in the Primary Literature," in *Data Handling for Science and Technology, An Overview and Sourcebook*, ed. Stephen A. Rossmassler and David G. Watson (Amsterdam: North-Holland Pub. Co., 1980), p. 68.

²⁰In May, 1982, a letter appeared in *Science* expressing dissatisfaction with the practice of storing experimental data in a remote depository. In particular the authors contended that the data were effectively unavailable to their students and colleagues during the course of research or experimental work when data are needed quickly. Furthermore, they believed that the cost of retrieving the data (a fee paid to the depository) and the time delay occasioned in corresponding with the depository inhibited or entirely prevented a scientist from quoting such data either in support of his own work for publication in a research journal or even in a review article or monograph. The authors specifically stated their preference for the publication of the data in miniprint form. Herbert Schumann and J. J. Zuckerman, "Omitted Data," *Science* 216 (21 May, 1982): 800.

Chapter 3

¹Walter H. Stockmayer, "Data Evaluation: A Critical Activity," *Science* 201 (18 August, 1978): 577.

²Lide, "Quality Control of Data," frame D-3.

³James R. Luedke, Jr., Gabor J. Kovacs, and John B. Fried, "Numeric Data Bases and Systems," *Annual Review of Information Science and Technology* 12 (1977): 122. See also CODATA Task Group on Accessibility and Dissemination of Data, p. 13, and Lide, "Quality Control of Data," frames D-3, D-4.

⁴CODATA Task Group on Accessibility and Dissemination of Data, p. 13.

⁵Ibid, p. 13.

⁶Howard J. White, "The National Bureau of Standards and the National Standard Reference Data System," in *A Review of AIChE's Design Institute for*

Physical Property Data (DIPPR) and Worldwide Affiliated Activities, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), p. 39.

⁷Luedke, p. 123.

⁸Ibid, p. 123.

Chapter 4

¹C. Y. Ho, "In Memoriam: Dr. Yeram Sarkis Touloukian," *Thermophysics and Electronics Newsletter* 10 (May/June 1981): 3-4.

²Maizell, p. 196.

³Wilhoit, "Thermodynamic Data Projects," p. 73.

⁴Ibid.

⁵Ronald P. Danner and Thomas E. Daubert, "The DIPPR Data Projects at the Pennsylvania State University," in *A Review of AIChE's Design Institute for Physical Property Data (DIPPR) and Worldwide Affiliated Activities*, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), pp. 8-10.

⁶David Zudkevich, "AIChE's DIPPR Experimental Program on Mixture Properties," in *A Review of AIChE's Design Institute for Physical Property Data (DIPPR) and Worldwide Affiliated Activities*, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), p. 59.

⁷Rosenfeld, 579-592, *passim*.

⁸J. D. Chase, "Activities of Fluid Properties Research, Inc.," in *A Review of AIChE's Design Institute for Physical Property Data (DIPPR) and Worldwide Affiliated Activities*, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), pp. 1-7.

⁹Beryl Edmonds, "Physical Property Data Service," in *A Review of AIChE's Design Institute for Physical Property Data (DIPPR) and Worldwide Affiliated Activities*, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), pp. 44-46.

Chapter 5

¹White, "The National Bureau of Standards," p. 39.

²National Research Council, *International Critical Tables of Numerical Data, Physics, Chemistry and Technology*, 7 vols. with index, prepared under the auspices of the International Research Council and the National Academy of Sciences, editor-in-chief, Edward W. Washburn (New York: McGraw-Hill, 1926-1933), p. xii.

³Weisman, "Needs for Property Data," p. 13. The first two sources were the *CRC Handbook of Chemistry and Physics* and *Chemical Abstracts*.

⁴CODATA Task Group on Accessibility and Dissemination of Data, p. 6.

⁵Tables de Constantes et Données Numériques. Tables Internationales de Constantes Sélectionnées, 17 vols. (vols. 1–5, Paris: Hermann; vols. 6–7, Paris: Masson; vols. 8–17, Oxford: Pergamon; 1951–1970). This series, with its variety of publishers, is further confused by the use of different titles for the overall series: “Tables of Constants of Numerical Data,” “International Tables of Selected Constants,” and “Physico-Chemical Selected Constants—New Series,” given in both French and English.

⁶*Tables of Physical and Chemical Constants and Some Mathematical Functions, 14th ed.*, originally compiled by G. W. C. Kaye and T. H. Laby, now prepared under the direction of an editorial committee (London: Longman, 1973).

⁷R. T. Bottle, “The Use of Standard Tables of Physical Data and Other Physicochemical Literature,” in *Use of Chemical Literature*, 3d. ed., ed. R. T. Bottle (London: Butterworths, 1979), p. 116.

Chapter 7

¹Maizell, p. 198.

²Dow Chemical Company Thermal Research Laboratory, *JANAF Thermochemical Tables*, 2d ed., D. R. Stull and H. Prophet, project directors, National Standard Reference Data Series, NSRDS-NBS 37 (Washington: U.S. Government Printing Office, 1971). For more information, see Part II, Chapter 2.

³A recent edition: Particle Data Group, “Review of Particle Properties,” *Reviews of Modern Physics* 52 (April 1980, part II): S1–S286.

⁴F. Ajzenberg-Selove, “Energy level of light nuclei $A=13-15$,” *Nuclear Physics A* 360 (4 May 1981): 1–186.

⁵International Union of Pure and Applied Chemistry, Inorganic Chemistry Division, Commission on Atomic Weights and Isotopic Abundances, “Atomic Weights of the Elements, 1979,” *Pure and Applied Chemistry* 52 (October 1980): 2349–2384.

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¹Public Law 176–56, Sec. 2, quoted in Raymond C. Cochrane, *Measures for Progress, a History of the National Bureau of Standards*, National Bureau of Standards Miscellaneous Publication 275 (Washington: U.S. Department of Commerce, 1966), p. 541.

²For an account of the first sixty years of work at NBS, see Cochrane, *Measures For Progress*.

³Ernest Ambler, “75 Years of Physics at NBS,” *Physics Today* (29 August 1976): 34–37.

⁴A complete account of this difficult period in NBS history, as well as information on the structure of NBS and its relationship to other parts of the federal government and to industry, is given in the Committee Print: Library of Congress, Congressional Research Service, Science Policy Division. *The National Bureau of Standards: a Review of its Organization and Operations, 1971-1980, a Study*, prepared for the Subcommittee on Science and Technology, U.S. House of Representatives, Ninety-Seventh Congress, First Session (Washington: U.S. Government Printing Office, 1981).

⁵Library of Congress, Congressional Research Service, Science Policy Division, pp. 1-2, 14, 20-21.

⁶NAS Evaluation Panel for the Center for Absolute Physical Quantities, *An Evaluative Report on the National Measurement Laboratory, National Bureau of Standards, Fiscal Year, 1979* (Washington: National Academy of Sciences, 1979), p. 28, cited in Library of Congress, Congressional Research Service, Science Policy Division, p. 20.

⁷H. H. Ku, *The Role of Standard Reference Materials in Measurement Systems*, National Bureau of Standards Monograph 148 (Washington: U.S. Government Printing Office, 1975).

Chapter 10

¹The official responsibilities of the System as first conceived by the Federal Council and the NBS were described by Edward L. Brady in *National Standard Reference Data System: Plan of Operation*, National Standard Reference Data Series NSRDS-NBS 1 (Washington: U.S. Government Printing Office, 1964).

²Public Law 90-396, quoted in Stephen A. Rossmassler, ed., *Critical Evaluation of Data in the Physical Sciences—a Status Report on the National Standard Reference Data System, January, 1977*, National Bureau of Standards Technical Note 947 (Washington: U.S. Government Printing Office, 1977), p. 30.

³Rossmassler, "Critical Evaluation of Data," p. 29; and Lide, "Quality Control of Data," frame D-1.

⁴Rossmassler, "Critical Evaluation of Data," p. 1.

⁵Ibid, p. 1.

⁶Lide, "Quality Control of Data," frame D-2.

⁷L. H. Gevantman, ed., *Physical Properties Data for Rock Salt*, National Bureau of Standards Monograph 167 (Washington: U.S. Government Printing Office, 1981).

⁸White, "National Bureau of Standards," p. 40; idem. "Standard Reference Data on Thermophysical Properties," in *Proceedings of the Seventh Symposium on Thermophysical Properties*, ed. Ared Cezairliyan (New York: American Society of Mechanical Engineers, 1977), p. 939.

⁹Rossmassler, "Critical Evaluation of Data," pp. 13-15; and Maizell, p. 188.

¹⁰Rossmassler, "Critical Evaluation of Data," p. 7.

¹¹Herman M. Weisman, "Technical Librarians and the National Standard Reference Data System," *Special Libraries* 63 (February, 1972): 69.

¹²Ibid, p. 74.

¹³Gertrude B. Sherwood, *Standard Reference Data Publications, 1964-80*, National Bureau of Standards Special Publication 612 (Washington: U.S. Government Printing Office, 1981).

Chapter 11

¹Cited by N. Kurti, "Capture, Evaluation and Storage of Data—as Seen by CODATA," *Pure and Applied Chemistry* 49 (1977): 1794.

²Kurti, pp. 1793-1795.

³International Council of Scientific Unions, Committee on Data for Science and Technology, *International Compendium of Numerical Data Projects: a Survey and Analysis* (Berlin: Springer-Verlag, 1969).

⁴It is of interest to observe the sparseness of this information for those data centers listed for the U.S.S.R. In the chapter for chemical kinetics only the names of three scientists and their addresses (but no telephone numbers) are given. Unlike the information for the remaining data centers (located in France, the Federal Republic of Germany, the United Kingdom, and the United States), there is nothing on the fields of specialization, the organizational structure (size, sponsors, number of staff), publications, or services available.

⁵M. L. Minges, "The CODATA Task Group on Transport Properties," in *Proceedings of the Seventh Symposium on Thermophysical Properties*, ed. Ared Cezairliyan (New York: American Society of Mechanical Engineers, 1977), pp. 943-944.

⁶J. H. Westbrook, "ICSU-CODATA Programs on Data for Industrial Needs," in *A Review of AIChE's Design Institute for Physical Property Data (DIPPR) and Worldwide Affiliated Activities*, ed. Stephen A. Newman, AIChE Symposium Series, no. 203 (New York: American Institute of Chemical Engineers, 1981), p. 24.

⁷CODATA Task Group on Fundamental Constants. *Recommended Consistent Values of the Fundamental Constants, 1973*, CODATA Bulletin, no. 11 (Frankfurt/Main: International Council of Scientific Unions Committee on Data for Science and Technology, 1973).

⁸*CRC Handbook of Chemistry and Physics*, 62nd ed. (Boca Raton, Florida: CRC Press, 1981), p. F-203.

⁹Richard E. Cohen and B. N. Taylor, "The 1973 Least-Squares Adjustment of the Fundamental Constants," *Journal of Physical and Chemical Reference Data* 2 (1973): 663-734.

¹⁰CODATA Task Group on Key Values for Thermodynamics, *CODATA Recommended Key Values for Thermodynamics*, CODATA Bulletin, no. 28 (Paris:

International Council of Scientific Unions Committee on Data for Science and Technology, 1978).

¹¹Idem, "CODATA Recommended Key Values for Thermodynamics, 1977," *Journal of Chemical Thermodynamics* 10 (October 1978): 903-906.

¹²The entry "Solubility" in NBS Special Publication 612, *Standard Reference Data Publications, 1964-1980*, which indexes all NSRDS publications, including all articles in the *Journal of Physical and Chemical Reference Data*, lists only three data compilations on solubilities: one on sparingly soluble lead salts, one on the mercury (I) chloride-water system, and one on selected metal hydrides. See also Chapter 10.

¹³"Solubility Data Series," *Chemistry International*, no. 5 (1980), p. 40.

¹⁴R. D. McCarty, "Thermodynamic Properties of Helium-4 from 2 to 1500 K at Pressures to 10^8 Pa," *Journal of Physical and Chemical Reference Data* 2 (1973): 923-1042. McCarty was given credit for his contribution on the title page of the IUPAC version, but it is unlikely that the U.S. taxpayer has been or will be reimbursed by Pergamon.

¹⁵*Chemistry International*, 1979, no. 3. Oxford: Pergamon Press, 1979-. Continues International Union of Pure and Applied Chemistry, *Information Bulletin*.

¹⁶White, "Standard Reference Data," p. 940.

¹⁷Heinrich Behrens and Gerhard Ebel, "Ein Informationsdienst über physikalische Daten in der Bundesrepublik Deutschland," *Nachrichten für Dokumentation* 29 (June 1978): 109-114.

¹⁸H. Behrens and G. Ebel, "Data Compilations in Physics," *Physik Daten/Physics Data*, no. 3-4 (1979), pp. 1-81.

¹⁹Hendrik van Olphen, "Numerical Data Advisory Board," *Bulletin of the American Society for Information Science* 1 (February 1975): 8 and passim.

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¹Judith Wanger and Ruth Landau, "Nonbibliographic On-line Data Base Services," *Journal of the American Society for Information Science* 31 (May 1980): 179.

²D. G. Watson, "Accessibility and Dissemination of Data," in *Data Handling for Science and Technology, an Overview and Sourcebook*, ed. Stephen A. Rossmassler and David G. Watson (Amsterdam: North-Holland Pub. Co., 1980), p. 135.

³Luedke, p. 143.

⁴Evan Buck, "The Industrial Data Bank: Utopia vs. the Real World," in *Phase Equilibria and Fluid Properties in the Chemical Industry*, ed. Truman S. Storvick and Stanley I. Sandler, ACS Symposium Series 60 (Washington: American Chemical Society, 1977), pp. 455-458; Wayne D. Dominick, "Numeric Data Base Systems: Concepts and Capabilities," in *The Value of Information*, papers

presented at the 6th mid-year meeting of the American Society for Information Science (N.p., 1977), pp. 55–60; Richard C. Simon, "Combined Online Numeric/Text Analysis and Retrieval Systems," in *Information * Politics, Proceedings of the ASIS Annual Meeting, 39th, 1976*, vol. 13. (Washington: American Society for Information Science, 1976), Part I, Abstracts, p. 71; and Randolph C. Wilhoit, "Design of a Multipurpose File of Thermodynamic Data," *Journal of Chemical Information and Computer Sciences* 20 (August 1980): 138–143.

⁵I. Eliezer, "Use of Computers in Handling of Laboratory Data," in *Data Handling for Science and Technology, an Overview and Sourcebook*, ed. Stephen A. Rossmassler and David G. Watson (Amsterdam: North-Holland Pub. Co., 1980), pp. 116–117.

⁶Lide, "Critical Data," p. 1347. Magnetic tapes for many NSRDS data compilations are available for sale by the National Technical Information Service.

⁷Donald T. Hawkins, "The ManLab-NPL Materials Data Bank," *Online* 3 (April 1979): 40.

⁸Wanger, p. 177.

⁹Bettijoyce Breen Molino, "Special Features of NBS's Omnidata System Applicable to the Retrieval, Analysis, and Dissemination of Chemical Data," *Journal of Chemical Information and Computer Sciences* 20 (August 1980): pp. 136–138.

¹⁰G. W. A. Milne and S. R. Heller, "NIH/EPA Chemical Information System," *Journal of Chemical Information and Computer Sciences* 20 (November 1980): 204–211.

¹¹Hawkins, pp. 40–43, 47–52.

¹²Helmut Knapp, "Centralized Service for Thermophysical Data in Germany—DSD: Dechema Data Service," in *Phase Equilibria and Fluid Properties in the Chemical Industry*, ed. Truman S. Storvick and Stanley I. Sandler, ACS Symposium Series 60 (Washington: American Chemical Society, 1977), pp. 459–467.

¹³John Nardone, "Computerized Numeric Data for Polymers," *Journal of Chemical Information and Computer Sciences* 19 (May 1979): 71–73; P. F. Roush, J. T. Seitz, and L. F. Young, "An On-Line System for Storage and Retrieval of Polymer Data," *Journal of Chemical Information and Computer Sciences* 19 (May 1979): 73–76; and Olga Kennard et al, "Computer Based Systems for the Retrieval of Data: Crystallography," *Pure and Applied Chemistry* 49 (1978): 1807–1816.

¹⁴IUPAC International Symposium on Techniques for the Retrieval of Chemical Information, London, 1976, "Main Lectures," *Pure and Applied Chemistry* 49 (1977), no. 12; and *Data for Science and Technology, Proceedings of the 7th International CODATA Conference, Kyoto, Japan, 1980*, ed. Phyllis S. Glaeser (Oxford: Pergamon Press, 1981).

¹⁵Joseph Hilsenrath, *Summary of On-Line or Interactive Physico-Chemical Numerical Data Systems*, National Bureau of Standards Technical Note 1122 (Washington: U.S. Government Printing Office, 1980).

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