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Stankus

Biographies of Scientists for Sci-Tech Libraries

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Adding Faces to the Facts

Tony Stankus
Editor

Biographies of Scientists for Sci-Tech Libraries: Adding Faces to the Facts

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Biographies of Scientists for Sci-Tech Libraries: Adding Faces to the Facts

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ABOUT THE EDITOR

Since 1974, Tony Stankus has run the Science Library at Holy Cross College, the Jesuit school of Worcester, Massachusetts. In that time he has also published over 30 papers and reviews, as well as *Scientific Journals: Issues in Library Selection and Management* (1987), *Scientific Journals: Improving Library Collections Through Analysis of Publishing Trends* (1990), *Making Sense of Journals in the Physical Sciences, and Making Sense of Journals in the Life Sciences* (both 1992), all from The Haworth Press, Inc. A study in the Fall, 1990, *College and Research Libraries* ranked him as second most productive author (among 1,373 compared nationally) of articles in journals of importance to academic librarianship in the 1980's. He has served on the editorial boards of *Library Acquisitions: Practice and Theory, Science and Technology Libraries*, and *RQ*, the Journal of the Reference and Adult Services Division of the American Library Association. He continues as column editor for "Sci-Tech Collections" in the second journal, and the "Alert Collector" in the last. When not working or writing, he raises vegetables which he claims have somehow been genetically engineered without his knowledge to account for his considerable girth. On Sundays he is to be found alongside his long forbearing wife, Mary Frances, at Saint Paul's Cathedral, the inner city Catholic parish where they serve together as lectors.

Spectra: A Bibliography of Sources

Gladys Odegaard
Julie M. Hurd

SUMMARY. Spectra are important sources of information about atoms and molecules. This paper surveys the various types of spectra and the nature of what each reveals about atomic or molecular structures or properties. The instrumentation employed is identified. A brief history of the development of spectroscopy is included as well as a bibliography of sources for additional reading on the topic.

The second part of this paper is an annotated bibliography of published sources for the major types of spectra. Scope and coverage of each source is noted as well as details on the nature of access to the spectral data.

PART I. SPECTRA AND SPECTROSCOPY: AN OVERVIEW

Early History of Spectroscopy

The earliest discoveries in spectroscopy were reported in writings on optics, as in the works of Sir Isaac Newton, Joseph Fraunhofer, and Robert Gustav Kirchhoff. Newton, whose work on spectra was first published in 1672, had wide-ranging scientific interests and for

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a number of years pursued a study of the fundamental nature of light. Newton invented a telescope and while working with lenses had produced a number of prisms. During experiments with a triangular prism which he had ground, he observed the dispersion of white light (from sunlight) into a multi-colored image—a spectrum. Other early spectroscopic experiments also represented efforts to understand and analyze light, frequently sunlight, but also that from incandescent sources such as flames. Fraunhofer, while engaged in work with lenses in the early nineteenth century, documented the dark lines that now bear his name interrupting the continuous spectrum of solar light. He published a detailed list of these lines by frequency and concluded that these were characteristic of sunlight. Some forty years elapsed before a partial explanation for these lines was provided by Kirchhof and Robert Bunsen who demonstrated a connection between the Fraunhofer lines and the spectra of metals. The fuller explanation that followed built on their work and ultimately attributed the dark Fraunhofer lines to absorption of light by the gaseous elements in the sun's atmosphere. This work provided the foundation for spectral analysis of distant astronomical objects and for the spectrochemical analyses now employed in countless scientific experiments. This early optical spectroscopy also led to techniques that allowed the testing of physicists' theories of atomic and molecular structure and led to a fuller understanding of atomic and molecular forces and energies.

Spectra as Information Sources

Atomic and molecular spectra are important information sources not only for chemists and physicists but for many other scientists who make use of the applications of spectroscopy to identify the presence of particular chemical species, whether in data returned from far-ranging space probes or from analyses of materials found within the human body or in core drillings from deep within the planet. Science and technology libraries frequently are visited by patrons seeking the spectra of known compounds or hoping to find in the published sources a spectrum that matches one they have measured. This article will describe some of the types of information that can be derived from spectra and will present an annotated

bibliography of some of the major sources of spectra. While a science information specialist can find it helpful to have studied spectroscopy, such a technical background is not essential in helping patrons to locate spectra they are seeking. The introductory remarks which follow here should provide a context in which the non-chemist can interpret queries about spectra and make most efficient use of the many compilations and indexes that provide spectral information.

What Are Spectra?

In the earliest years of its history the term "spectrum" referred to the range of wavelengths perceived as colors of light by the human eye. As techniques and instrumentation developed, usage broadened to signify the entire range of electromagnetic radiation. In fact, the field now encompasses mass spectrometry as well where, rather than radiation emitted or absorbed, the instrumentation measures the distribution of charged particles produced after ionization of the sample.

Spectroscopy is an analytical technique that measures the interaction of energy with matter. As it is currently practiced, spectroscopy utilizes complex instrumentation to make and record these measurements—*spectra*—which are then interpreted to provide practical information such as definitive identification of the presence of specific atoms or molecules or to serve as the basis for theoretical discussions of the fundamental physical structure of chemical species. The practical applications of spectroscopy are widespread and used in many branches of pure and applied science and engineering. An understanding of the theoretical aspects of spectroscopy makes use of quantum mechanics and is a highly mathematical area of study pursued by physical chemists and chemical physicists. Many users of spectral data do so without this depth of understanding and, at some levels of application, are not handicapped by this lack.

A display of the data collected from a spectroscopic measurement is called a *spectrum*. A spectrum may be represented as a plot of intensity of radiant energy emitted or absorbed (or some function of intensity) versus the energy of that radiation (typically displayed as

wavelength or frequency). Alternatively, a spectrum may be recorded as a series of numbers (representing emission or absorption peaks) that convey comparable information. Each chemical entity possesses its own unique spectrum. A spectrum may be thought of as the "fingerprint" of a species and it is frequently used in chemical analysis work as the basis for identification just as fingerprints are used to identify persons. Spectra can convey both qualitative information, i.e., the presence of a species, or quantitative information, i.e., the relative amounts of components in a mixture.

Types of Spectra

Spectra are classified (and sometimes named) according to type of radiation emitted or absorbed. Electromagnetic radiation is characterized by its wavelength which can vary from extremely long but low energy, as in the case of radio or microwaves, through the infrared and visible regions of the spectrum to very short wavelengths at the high-energy end of the spectrum as in X-rays or gamma radiation. (The energy of the radiation is inversely proportional to the wavelength.) Table 1 displays the principal regions of the electromagnetic spectrum and shows the units most conveniently used to measure wavelengths in each region. Each type of spectrum provides information on atomic or molecular energy levels, the distribution of species among energy levels, molecular geometries, chemical bonding, or interactions among molecules in mixtures or solutions. See Table 2 for the principal spectral regions, the instrumentation commonly employed in each, and the types of atomic or molecular transitions occurring in each region.

In the radio frequency and microwave regions of the spectrum the transitions observed relate to changes in either molecular rotational energy levels, nuclear spin levels (nuclear magnetic resonance or NMR), or electron spin levels (electron spin resonance or ESR). Both NMR and ESR spectroscopy measure the effects of magnetic fields on a sample. *Electron spin resonance spectroscopy* (also known as *electron paramagnetic resonance spectroscopy* or EPR) is concerned with the absorption of radiation by electrons in a molecule. ESR spectra can provide information on electronic structure and chemical reaction kinetics for paramagnetic species[1] including

FIGURE 1
The Electromagnetic Spectrum[1]

Spectral Region	Approximate Wavelength Range
Radio-frequency	10^{1} - 10^{3} meters (m)
Microwave	0.1 - 30 centimeters[2] (cm)
Infrared	2.5 - 50 micrometers[3] (μm)
Visible	400 - 800 nanometers[4] (nm)
Ultraviolet	200 - 400 nm
X-ray	0.05 - 1 nm
Gamma	< 0.05 nm

[1] McGraw-Hill Encyclopedia of Science and Technology, 6th edition. New York: McGraw-Hill; 1987. See the article on "spectroscopy," volume 17, pages 213-219.

[2] 1 cm = 10^{-2}m

[3] 1 μm = 10^{-6} m

[4] 1nm = 10^{-9} m = 10 angstroms (Å)

FIGURE 2

Principal Types of Spectra[1]

Spectral Region	Radiation Source	Detector	Transitions
Radio-frequency	Radio transmitter	Radio receiver	Molecular rotations, nuclear magnetic resonance (NMR)
Microwave	Klystron	Silicon-tungsten crystal	Molecular rotations
	Magnetron	Bolometer	Electron Spin Resonance (ESR)
Infrared	Nernst glower	Thermocouple	Molecular vibrations
	Globar lamp	Bolometer	
Visible	Tungsten lamp	Photocell	Electronic excitation (atomic)
Ultraviolet	Hydrogen-discharge lamp	Photomultiplier	Electronic excitation (molecular)
X-ray	X-ray tube	Geiger counter	Ionization
Gamma	Radioactive nuclei	Geiger counter	Nuclear transitions and disintegrations
		Scintillation Counter	

[1] McGraw-Hill Encyclopedia of Science and Technology. 6th edition. New York: McGraw-Hill; 1987. See the article on "spectroscopy," volume 17, pages 213-219.

biological molecules, metals, complexes, and others whether in solid, liquid or gas phase. The technique is non-destructive and finds applications in solid state physics, organic and inorganic chemistry, materials science, biology, and environmental science.

Nuclear magnetic resonance spectroscopy originates from the effect of a magnetic field on atomic nuclei, most frequently either protons (i.e., ^{1}H) or ^{13}C. NMR spectroscopy has been used to elucidate structures of compounds important in numerous disciplines and has recently been developed as a non-invasive medical procedure that provides images of living organisms. This latter application is known as *magnetic resonance imaging* or MRI and is rapidly becoming a standard diagnostic device, especially in the area of cancer detection.

Microwave spectroscopy detects transitions between rotational energy states of molecules and, after analysis, offers data on molecular geometries, i.e., bond lengths and bond angles. The earliest work provided structural parameters for relatively low molecular weight organic species but the technique has more recently been extended to provide information on complex biologically-significant compounds as well as for free radicals and other unstable species.

Infrared spectra (IR) originate from vibrations (stretching, bending, rocking, etc.) of the bonds in molecules. Infrared spectroscopy provides information on functional groups present and their spatial arrangements that are of interest to scientists in many fields including chemistry, materials science, environmental science and engineering. Until the development of NMR spectroscopy in the 1950's, IR spectroscopy was the most important analytical technique for identification of species. It has seen a resurgence of interest with the development in the 1970's of *Fourier transform infrared spectroscopy* (FT-IR) and new commercially-available instrumentation that supports use of the technique in routine analyses. This type of spectrum, more than any other, is considered a molecular "fingerprint."

Raman spectra provide information on molecular vibrations and/or rotations complementary to that obtained from infrared spectra. Lasers are utilized as the source of radiation in the far infrared-

visible region. This technique can be used to study metal bonding, ring compounds, steroids, and long chain molecules, among others.

Emission spectra observed in the *visible* region were among the earliest to be studied. They may be continuous spectra as emitted by incandescent solids, line spectra emitted by excited atoms, or band spectra emitted by excited molecules. The methods provide both quantitative and qualitative data for identification and analysis.

Ultraviolet (UV) and *visible* absorption spectra result from electronic transitions in molecules that produce broad bands best suited for qualitative study of simple solid or liquid samples whose molecules contain "chromophores"—structural fragments that absorb radiation at characteristic frequencies in this region. The spectrum obtained provides information on groups present or not present in the sample and is a function of the whole structure of the substance.

X-rays can cause substances to emit electrons and the energy distribution of these particles is a photoelectron spectrum which provides information on the electronic structure of the sample. In similar fashion *gamma rays* reveal details of nuclear structure.

Mass spectrometry is a destructive technique that separates gas phase ions produced from the sample being analyzed according to their masses or ratios of charge to mass. The resulting distribution of species resembles the spectra that are produced by emission or absorption of electromagnetic radiation and so the technique is frequently considered to be spectroscopic in nature; the terminology employed and the classification of library materials reflects that perspective. Mass spectrometry supports the identification of atomic and molecular chemical species even at the level of resolution that separates various isotopes of an element. This technique is another "fingerprint" procedure with many analytical applications. For these reasons sources of mass spectra are included in this bibliography.

Instrumentation

The types of instruments used to measure and record spectra are known variously as spectrometers, spectrophotometers, spectrographs, or spectroscopes and which instrument or term is employed in a given measurement depends on the spectral region. The process

of recording a spectrum can be depicted schematically as shown in Figure 1. In any spectrometric experiment the sample (the species whose spectrum will be measured) must be properly prepared so as to interact with the radiation to which it will be subjected. This preparation may be simple, as in cases where the compound need only be placed in a suitable container (IR spectroscopy), or it may be more involved, even to the extent of decomposing a compound into its constituent atoms (mass spectrometry).

For absorption spectra, the prepared sample is subjected to electromagnetic radiation which is absorbed by the sample with a resultant increase in energy. Radiation not absorbed passes through the sample to a resolving device which separates the wavelengths present and allows a detector to analyze the intensity of radiation at each wavelength. The plot of intensity versus wavelength is an absorption spectrum and it displays lower intensities of transmitted radiation that correspond to the energy absorbed by the sample.

Emission spectra are obtained by employing an external energy source (heat, magnetic, mechanical, etc.) to raise the energy level of the sample. After the external source is removed, the sample then emits the energy gained as radiation: an emission spectrum. This emitted radiation passes through the resolving device and the measurement system. Recorded emission and absorption spectra, as noted above, are sources of both quantitative and qualitative information. The particular combination of wavelengths emitted or absorbed can reveal the presence of a specific chemical entity (qualitative); the intensity of the radiation provides information of a quantitative nature after suitable analysis.

As each of type of spectroscopy developed, the earliest instruments were built by those scientists who were the first to study that particular spectral region. As a specialization developed further, the instrumentation became commercially available, much in the same fashion as turn-key library automation systems followed individually-developed systems. Just as turn-key systems made it possible for more libraries to automate their activities, so commercially available spectroscopic equipment broadened the usage of spectroscopic techniques. Laboratories not directly involved in fundamental research in spectroscopy could purchase and use equipment that allowed increasingly sophisticated analyses of chemicals. These in-

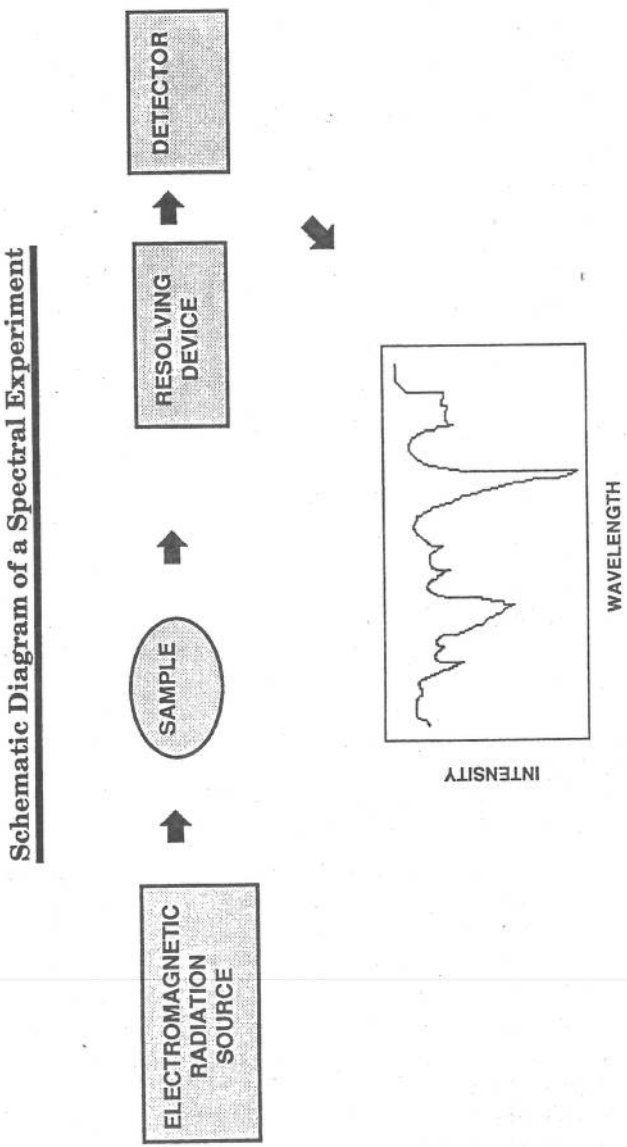

FIGURE 3
Schematic Diagram of a Spectral Experiment

strumental techniques frequently replaced analytical techniques that utilized diagnostic reactions to identify chemicals present or quantitative methods employed to analyze multi-component mixtures. In turn, these new applications diversified the users of collections of spectra from the original chemists and physicists to include biologists, medical researchers, engineers and others. This fact should be recognized by information specialists working with materials on spectra because it may be important for a library to provide supplemental resources to assist some users of spectra collections. For example, a specialist in materials science may require guidance in identifying the systematic name for a chemical which is known in her laboratory only by its trade name.

Uses and Users of Spectra

Science library patrons seeking spectra or information about spectroscopy may range from the undergraduate chemistry student with a lab experiment in process to the research scientist seeking to identify a newly isolated compound. The library resources these patrons might consult could include introductory materials on spectroscopy to supplement a course text, organized compilations of published spectra, or the research literature in journals and technical reports. This article will suggest a few sources of introductory information to assist users in understanding spectra but will concentrate primarily on describing a selection of the numerous compilations of spectra. It must be noted here, however, that these are not exhaustive sources. As voluminous as several of the published collections are, not all compounds known are represented. There are many species whose spectra have not been measured or, if measured, may be found only in a journal article or in records of the scientist who determined the spectrum. Even the most skilled literature searcher may not be able to locate a sought-after spectrum; it may not be published and waiting to be found. It is the goal of this article to provide a list of sources sufficiently comprehensive that the search may be as exhaustive as available resources can support. After consulting without success the compilations listed in this article, a search of *Chemical Abstracts,* Beilstein[3] (for organic compounds), or Gmelin[4] (for inorganic compounds) may be required

before it can be said with confidence that a published spectrum is not available. Searching these specialized reference sources will not be covered in this article as that is a topic deserving of fuller consideration and which is treated in a number of guides to the chemical literature.

Using Compilations of Spectra

There are certain features common to many of the compilations listed in the bibliography provided in Part II and these will be summarized here. As with any other reference work, these are best approached on first use by a careful examination of the introductory material. There one will usually find information on the scope and coverage of the work: what kind of spectra are included, for what type of compounds, taken from what sources, and arranged in what sort of order. The reader may also learn whether the compilation is an ongoing one that will be updated and, if so, with what regularity. It is essential to know what kind of access is provided to the spectra in a particular work. Some of the possibilities include: chemical name (common, trade, or systematic), chemical formula, molecular weight, major peaks or absorption lines, and Chemical Abstracts Service Registry Number. If a compilation is a multi-volume set, there may be cumulative indexes; if these do not exist it may be necessary to search individual volume indexes.

Information describing a compilation of spectra is not always easily found in its prefatory material. The extent to which an information specialist can learn about the features of a compilation influences the perceived utility of the reference in application to a specific problem. Put simply, if a scientist has only a spectrum and a chemical formula, those indexes with a chemical formula index and/or a listing of principle peaks are likely to offer a better beginning than those organized solely by chemical name. Conversely, the patron seeking a spectrum of a particular compound might best be referred to those works that provide chemical name or registry number indexes. In the bibliography that follows in the second part of this article the citations are annotated with information on scope, types of indexes, etc. to guide the users of those sources.

There are several publishers known for their very comprehensive

compilations of spectra which are among those listed in the bibliography in part II. The Aldrich Chemical Company publishes spectral collections (*libraries*) that are organized by chemical categories based on chemical structures. Their libraries include NMR spectra, infrared spectra, Fourier Transform infrared spectra (FT-IR), and a carbon-13 NMR set. In addition, they offer a set of microfiche indexes to seven physical properties for Aldrich chemicals. All the compounds included in their publications are commercially available from the company. Indexes to spectral libraries typically include chemical name, molecular formula and CAS Registry Number. Full chemical names are provided for each species rather than trade names as are sometimes used in other sources. Because their inventory is extensive, the Aldrich collections can provide an easy-to-use first reference that offers a high probability of success for many chemicals.

The Sadtler Research Laboratories in Philadelphia have been publishing collections of spectra since 1947. Their comprehensive collections include over 342,000 spectra organized by type of spectra, UV, IR, NMR, ^{13}C NMR, Raman, etc., and the ongoing collections are issued in looseleaf binders of a particular shade of dark green well-known to users of their data. Their libraries are typically indexed by name, chemical formula, and chemical structure or group and use a Sadtler spectrum number as the basis for organization of the individual spectra. Sadtler also publishes a collective index to their entire set. In addition to the print format, machine-readable data for use with particular instruments or personal computers is also available. For those seeking a spectrum for a known compound, these comprehensive compilations promise a good chance of success.

Another publisher of specialized sources on spectra has been the American Petroleum Institute (API) which began in 1941, in cooperation with the National Bureau of Standards, to assemble data on physical, chemical, and spectral properties of hydrocarbons and other compounds of interest to the petroleum industry. The API Project 44 has grown over the years and is now located at the Thermodynamics Research Center (TRC) associated with Texas A & M University.

The sources of spectral information published by the above labo-

ratories and others included in the bibliography that follows have appeared in book format, often in looseleaf binders that allow for additions of new spectra as these become available. Microform versions also have been available and are a more space-conserving storage medium. In recent years compilations of spectra have also begun to appear in machine-readable form supporting retrieval and manipulation of the data. These databases of spectra are likely to increase in number and size and very likely represent the future format for this type of information.

Books About Spectra

Listed here are books about spectra and spectroscopy that complement the sources of spectra themselves found in Part II of this paper. These materials range from very introductory level reference works that might be useful to undergraduate students to monographs used as course texts in graduate courses that teach about spectroscopy. It should be noted that only a very small selection of the latter type of work is included here; the titles listed have been chosen because they are among the more recent books published on the topic and may be less well-known than some of the classic works in the field. They serve as examples of a much larger body of literature. Additional introductory reading may also be found in any good scientific encyclopedia under entries such as "spectra," "spectroscopy," and the various types of spectra.

Acronyms and abbreviations in molecular spectroscopy. Detlef A.W. Wendisch. Berlin and New York: Springer-Verlag; 1990. 315 pages. Entries include definitions, applications, and literature references.

Analytical instrumentation handbook. Galen Wood Ewing, editor. New York and Basel: Marcel Dekker; 1990. 1071 pages. Chapters contributed by various analytical chemists describe instrumentation and techniques. Illustrations and bibliographies.

A Bibliography of matrix isolation spectroscopy: 1954-1985. David W. Ball et al. Houston, TX: Rice University Press; 1988. 643 pages. Bibliography of published references that deal with matrix-isolation spectroscopy with emphasis on cryogenic inert gas

matrix isolation. Almost 3700 items in 3 section: Books, review articles, general references. Author, subject and formula indices.

The chemist's ready reference handbook. Gershon J. Shugar and John A. Dean, consulting editors. New York: McGraw-Hill; 1990. various paging. Describes instrumentation and analytical procedures in chapter arrangement with references and bibliographies.

[*CRC*] *Handbook of spectroscopy.* J.W. Robinson, editor. Boca Raton, FL: CRC Press; 1974. 2 volumes. Intended to provide a reference for the spectroscopic data available on the most important materials in the major fields of spectroscopy.

A dictionary of concepts in NMR. S.W. Homans. Oxford: Clarendon; 1989. 343 pages. "The aim . . . is to aid chemists and biochemists familiar with the basic principles . . . to understand the bewildering array of acronyms and technical jargon . . ." Biased towards two-dimensional NMR methods in liquids. Many entries include references for further reading.

A dictionary of spectroscopy. Ronald Denney. 2d edition. New York: Wiley; 1982. 205 pages. The most common expressions, equations and terms in an alphabetical format with literature references. Includes modern and traditional types of spectroscopy. Directed to students and those not generally familiar with developments in the field.

The encyclopedia of spectroscopy. George C. Clark, editor. New York: Reinhold; 1960. 787 pages. Topics arranged alphabetically according to principal kinds of spectroscopy and then by the various aspects. Signed articles.

Fundamentals of molecular spectroscopy. 2d edition. C.N. Banwell. New York and London: McGraw-Hill; 1972. 332 pages. Non-mathematical introductory treatment.

Fundamentals of molecular spectroscopy. Walter S. Struve. New York: Wiley; 1989. 379 pages. Introduction to spectroscopy of atoms and molecules for graduate students with some background in quantum mechanics and mathematics.

Group theory in spectroscopy: with applications to magnetic circular dichroism. Susan B. Piepho and Paul N. Schatz. New York:

Wiley; 1983. 634 pages. Advanced treatment of application of group theoretic methods to molecular spectroscopy.

A guide to collections and indexes of spectra. Irwin A. Rodin, compiler. Waterloo, ON: University of Waterloo. Engineering, Mathematics and Sciences Library; 1978. 25 pages. Annotated bibliography of collections of spectra and indexes to spectra in the EMS Library; will help locate spectra by name, formula, wavelength, shift, mass/charge or functional group.

Mass spectrometry: applications in science and engineering. Frederick A. White and George M. Wood. New York: Wiley; 1986. 773 pages. Interdisciplinary overview of modern mass spectrometry with historical background, instrumentation, and applications in engineering, physical sciences and life sciences.

Molecular spectroscopy. Jack D. Graybeal. New York: McGraw-Hill; 1988. 732 pages. Provides a foundation for beginning graduate students seeking a quantum mechanical treatment of molecular spectroscopy including rotational, vibrational, and electronic spectra as well as nuclear and electron resonance.

Molecules and radiation: and introduction to modern molecular spectroscopy. Jeffrey I. Steinfeld. Cambridge, MA and London: MIT Press; 1979. 348 pages. Graduate level introduction for chemical physics students to modern molecular spectroscopy intended to provide background for understanding of current research in the field.

Multilingual dictionary of important terms in molecular spectroscopy. International Union of Pure and Applied Chemistry. Commission on Molecular Structure and Spectroscopy. Ottawa: National research Council of Canada; 1966. 221 pages. English, French, German, Japanese and Russian.

Nineteenth Century Spectroscopy: Development of the Understanding of Spectra 1802-1897. William McGucken. Baltimore and London: Johns Hopkins,1969. 233 pages. Examines developments from the work of Wollaston with dark solar lines (1802) through discoveries by Busen and Kirchhof in 1860 up to J.J. Thomson's discovery of the electron in 1897.

Spectrometric identification of organic compounds. 4th edition. Robert Silverstein, G. Clayton Bassler and Terence C. Morrill. New York: Wiley; 1981. 442 pages. A how-to-do-it book. Identifications by means of mass, IR, NMR and UV spectroscopy.

Symmetry and spectroscopy: an introduction to vibrational and electronic spectroscopy. Daniel C. Harris and Michael D. Bertolucci. New York: Oxford; 1978. 550 pages. Introductory level text for upper level undergraduate and beginning graduate level chemistry students. Begins with chapter on group theory. Many examples and experimental results.

PART II. BIBLIOGRAPHY

This bibliography lists collections of spectra and indexes to spectra grouped by type of spectra and organized within each group alphabetically by title. Sources of spectra in the visible region may be found in the sections on infrared and ultraviolet spectra, or in the section on "miscellaneous and various spectra," depending on how material was organized by source's compiler. This bibliography is based on the Spectra Collection maintained by the Science Library at the University of Illinois at Chicago and represents selected sources from that collection. The authors welcome suggestions of items that might be added to this compilation or information on new editions of sources included here.

Carbon-13 NMR Spectra

Atlas of carbon-13 NMR data. E. Breitmaier, G. Haas and W. Voelter. London, Philadelphia: Heyden; 1979. 3 volumes. Lists 1,003 organic compounds. Does not include spectra. Indexed alphabetically, by IUPAC name, chemical class, molecular formula, molecular weight, and chemical shift.

Carbon-13 NMR spectra; a collection of assigned, coded, and indexed spectra. Leroy F. Johnson and William C. Jankowski. Huntington, NY: R.E. Krieger; 1978. 580 pages. 500 spectra arranged in empirical formula order. Indexed by name, code (a cod-

ing system similar to that in the Varian proton NMR catalogs was used), and chemical shift.

Chemical shift ranges in carbon-13 NMR spectroscopy. Wolfgang Bremser, Burghard Franke and Hans Wagner. Weinheim, Deerfield Beach, FL: Verlag Chemie; 1982. 890 pages. Lists expectation ranges of chemical shifts and functions of partial structures; provides a means of predicting the positions of the C-13 NMR signals of almost any given structure. Printed version of the file from the COM-Microfiche collection Carbon-13 NMR spectral data published by Verlag Chemie. 23,450 compounds; about 240,000 shifts corresponding to 100,000 different substructure codes.

Sadtler guide to carbon-13 NMR spectra. William W. Simons, editor. Philadelphia: Sadtler Research Laboratories; 1983. 652 pages. A survey collection of 500 selected spectra with emphasis on chemical shifts. Ordering by functional groups, similar to other Sadtler handbooks. Alphabetical, numerical and molecular formula indexes.

Selected ^{13}C nuclear magnetic resonance spectral data. American Petroleum Institute. Research Project 44. College Station, TX: Thermodynamics Research Center, Texas A & M University; 1974-. Principally hydrocarbons and compounds of interest to the petroleum industry Indexed; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

Standard carbon-13 NMR spectra. Philadelphia: Sadtler Research Laboratories; 1980-. 16 mm reel-to-reel microfilm or looseleaf. Spectra only. 19,000 spectra as of 1985. Indexed by *Standard carbon-13 NMR spectra collection indexes.*

Infrared Spectra

Absorption spectra in the infrared region. L. Lang, editor. London: Butterworths (volumes 1-2) and Huntington, NY: R.E. Krieger (volumes 3-4); 1974-78. 4 volumes.

Organic compounds of interest to the pharmaceutical and petrochemical industries. Volumes are individually indexed by substance, formula and author; each also includes list of literature references.

The Aldrich library of FT-IR spectra. Charles Pouchert. Milwaukee: Aldrich Chemical Company: 1985. 2 volumes.

Spectra for 11,000 compounds. Alphabetical, molecular formula and CAS registry number indexes.

Aldrich library of infra-red spectra. Charles Pouchert. 3rd edition. Milwaukee: Aldrich Chemical Company; 1981. 1873 pages.

Contains 12,000 spectra arranged by functional group in an order of increasing complexity.

Alphabetical and molecular formula indexes.

Atlas of infrared spectroscopy of clay minerals and their admixtures. H.W. van der Marel and H. Brudelspacher in collaboration with E. Reitz and P. Krohmer. New York: Elsevier; 1976. 396 pages.

Examples selected from about 4,000 samples totally investigated, most from well-known localities. Includes spectra. Extensive bibliography and subject index.

Atlas of polymer and plastics analysis. Dieter O. Hummel and Friederich K. Scholl. 2d, revised, edition Munich: Hanser and Weinheim: Verlag Chemie; 1978. 5 volumes.

V.1: Polymers: structures and spectra.—v.2: Plastics, fibres, resins: starting and auxiliary materials, degradation products.—v.3: Additives and processing aids. Spectra arranged by structure class with name and formula indexes. Bibliography.

ATR; attenuated total reflectance. Philadelphia, PA: Sadtler Research Laboratories; 1966-. Looseleaf.

1500 attenuated total reflectance spectra of commercially available monomers and polymers; volumes 1-2 are prism spectra, volumes 3-5 are grating spectra. Precise listing of chemical categories in introduction to index. Alphabetical index by trade name, and chemical name where applicable: chemical classification by type.

Evaluated infrared reference spectra (the Coblentz Society spectra). Joint Committee on Atomic and Molecular Physical Data. Printed and distributed by Sadtler Research Laboratories, Philadelphia, PA; 1961-. Looseleaf.

10,500 spectra. Indexed by spectrum number, name and molecular formula.

Handbook of infrared standards, with spectral maps and transition assignments between 3 and 2600 μm. Guy Guelachvili and K. Narahari Rao. Orlando, FL: Academic Press; 1986. 851 pages.

"It has long been recognized that one can make full use of the high resolution achieved in IR spectra only when there is corresponding precision available in the wavenumber standards used for calibrations. . . . This handbook provides lists of IR standards based on spectra of easily available molecular species . . ." – Introduction. Spectral maps, wavenumber tables, and transition assignments for CO, OCS, CO_2, N_2O, H_2O, $^{14}NH_3$, $^{15}NH_3$, and C_2H_4.

Index of vibrational spectra of inorganic and organometallic compounds. Norman N. Greenwood, E.J.F. Ross and B.P. Straughan. London: Butterworths: 1972. 3 volumes.

Approximately 25,000 compounds (IR and Raman). Spectra not included. Formula index.

Infrared absorption spectra; index, 1945-1957. H.M. Hershenson. New York: Academic Press; 1959. 111 pages.

Bibliographic references for spectra of 16,000 organic and inorganic compounds. Does not include spectra. Chemical substance index.

Infrared analysis of polymers, resins and additives: an atlas. Dieter O. Hummel and Friederich K. Scholl. New York: Wiley-Interscience; 1969. 2 volumes.

Part. 1: Text; Part. 2: Atlas. 1,774 compounds. Includes spectra. Chemical substance index.

Infrared band handbook. Herman Szymanski and Ronald E. Erickson. 2d edition, revised and enlarged. New York: IFI/Plenum; 1970. 2 volumes.

27,840 IR bands of organic and inorganic compounds. Does not include spectra. Formula index.

Infrared spectra and characteristic frequencies ~ 700-300 cm^{-1}. Freeman Bentley, Lee D. Smithson and Adele L. Rozek. New York: Interscience; 1968. 779 pages.

1,566 organic and inorganic compounds. Includes spectra. Formula index.

The infrared spectra atlas of monomers and polymers. Philadelphia, PA: Sadtler Research Laboratories; 1980. 810 pages.

Desk reference collection of 2000 IR reference spectra of monomers, polymers and precursors commonly encountered in industry and academia. Spectra are arranged into chemical class and in order of increasing complexity within each class. Alphabetical, numerical and Spec-Finder indexes.

The infrared spectra atlas of surface active agents. Philadelphia, PA: Sadtler Research Laboratories; 1982. 846 pages.

Reference collection of 2000 IR spectra of surface active agents encountered in both industry and academia. Substances identified by commercial names and chemical or descriptive names. Numerical, alphabetical and Spec-Finder indexes.

Infrared spectra handbook of common organic solvents. Philadelphia, PA: Sadtler Research Laboratories; 1983. 400 pages.

Infrared reference spectra of 400 common solvents grouped by chemical class, presented in a transmittance vs. frequency (wave number) format over the spectral region 4000-400 cm^{-1}. Alphabetical and molecular formula indexes.

The infrared spectra handbook of inorganic compounds. Philadelphia, PA: Sadtler Research Laboratories; 1984. 345 pages.

A desk reference collection of infrared spectra for 345 inorganic compounds, compiled by Sadtler Research Laboratories. Also includes pertinent chemical and physical data; alphabetical and molecular formula indexes.

The infrared spectra handbook of priority pollutants and toxic chemicals. Philadelphia, PA: Sadtler Research Laboratories; 1982. 727 pages.

564 IR reference spectra representing 363 chemical substances which have appeared in the EPA Priority Pollutants List, the OSHA Category I List of Carcinogenic Substances and a list of hazardous compounds are common to industry and of concern during interstate transportation. Some 200 of the compounds are represented by both condensed phase and vapor phase spectra. Compiled by Sadtler Research Laboratories. Alphabetical, molecular formula and Spec-Finder indexes.

Infrared spectra of inorganic compounds (3800-45 cm^{-1}). Richard Nyquist and Ronald O. Kagel. New York: Academic Press; 1971. 495 pages.

892 compounds. Includes spectra. Chemical substance index.

Infrared spectra of minerals and related inorganic compounds. J.A. Gadsden. London: Butterworths; 1975. 277 pages.

Contains IR band tables for over 600 minerals and 100 other related inorganic compounds, referenced to the literature where the original spectra can be found. Also includes references to a further 550 minerals and inorganic compounds. Subject/chemical and mineral indexes.

Infrared vapour spectra, group frequency correlations, sample handling and the examination of gas chromatographic fractions. David Welti. London: Heyden, in cooperation with Sadtler Research Laboratories: 1970. 211 pages.

Includes 306 vapor spectra in numerical serial order, with index to vapor spectra in Sadtler, DMS, Coblentz and Wyandotte systems.

Inorganics and related compounds. Philadelphia, PA: Sadtler Research Laboratories; 1967-. Looseleaf.

1300 spectra of organic and coordination compounds. Alphabetical and numerical indexes.

Interpretation of vapor-phase infrared spectra. R.A. Nyquist. Philadelphia, PA: Sadtler Research Laboratories; 1984. 2 volumes.

Intended to aid in the interpretation of vapor phase infrared spectra generated utilizing the gas chromatography/infrared technique. Vol. 1: Group frequency data; Vol. 2: Spectra (500 vapor phase IR reference spectra). Alphabetical and molecular formula indexes.

Lubricants; grating spectra. Philadelphia, PA: Sadtler Research Laboratories; 1966-. Looseleaf.

900 spectra. Alphabetical and class indexes.

Massachusetts Institute of Technology wavelength tables. Cambridge, MA: Massachusetts Institute of Technology. Spectroscopy Laboratory; 1939. 2 volumes.

Main tables contain more than 100,000 entries for the most important known spectrum lines emitted between 10,000 and 2000

angstroms by atoms in the first two stages of ionization. – Introduction. Emission lines measured by diffraction-grating spectrographs.

Massachusetts Institute of Technology wavelength tables. Volume 2: Wavelengths by element. Massachusetts Institute of Technology. Spectroscopy Laboratory. Cambridge, MA: MIT Press; 1982.

First stage of a project to expand and correct the 1939 edition. Presents the same atomic emission lines (as corrected in the 1969 edition) rearranged by element, with the addition of wavelengths in vacuum.

Molecular spectra of metallic oxides. Alois Gatterer, J. Junkes and E.W. Salpeter. Citta del Vaticano: Specola Vaticano; 1957. 91 pages.

Wavelength tables; portfolio of 36 plates. Principally spectra of astrophysical interest. Spectral range from 9000 to 2000 Å; grating spectrograph. Organized by compound. Analytical remarks rely heavily on Rosen's *Données spectroscopiques concernant les molecules diatomiques* published in 1951.

Pharmaceuticals grating spectra. Philadelphia, PA: Sadtler Research Laboratories; 1972-. Looseleaf.

1200 spectra. Indexed by name, molecular formula, and therapeutic application.

Standard grating spectra. Philadelphia, PA: Sadtler Research Laboratories; 1968-. Looseleaf.

79,000 spectra by 1990. Indexed through the *Sadtler cumulated comprehensive indexes.*

Sadtler handbook of infrared spectra. William W. Simons, editor. Philadelphia, PA: Sadtler Research Laboratories; 1978.

Abridged edition (approximately 3,000 spectra) of *Sadtler standard IR grating spectra.* 1035 pages.

Intended to serve as a small, convenient reference collection of IR spectra of organic compounds for college courses or when comprehensive collections are not available.

Sadtler infrared spectra handbook of esters. Philadelphia, PA: Sadtler Research Laboratories; 1982. 686 pages.

The term 'esters' as used to describe the contents of this volume

is applied only to the non-cyclic esters of carboxylic acids. Other types of esters will appear in future volumes dedicated to that group of compounds, e.g., sulfonic acid esters will be included with other compounds containing sulfur. 2,000 IR grating spectra selected from among those published in the *Standard IR grating collection* between 1966 and 1980. Alphabetical, Spec-Finder and numerical indexes.

Sadtler infrared spectra handbook of minerals and clays. John R. Ferrar, editor. Philadelphia, PA: Sadtler Research Laboratories; 1982. 440 pages.

A collection of 400 infrared spectra of various minerals taken in the region of 4000-250 cm^{-1}, determined using the KBr pellet technique. Presented in a linear transmittance vs. wave number format; classified according to an increasing order of complexity of the mineral. Indexed alphabetically by name of mineral.

Selected infrared spectral data. American Petroleum Institute. Research Project 44. Washington, DC: American Petroleum Institute, 194-. 2 volumes. Looseleaf.

Principally hydrocarbons and compounds of interest to the petroleum industry. 3,395 compounds through 1976. Indexed; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

Tabulation of infrared spectral data. David Dolphin and Alexander Wick. New York: Wiley; 1977. 549 pages.

Changes in characteristic group frequencies. Does not include spectra, except for spectra of common solvents given in the last chapter. Wave number-micron conversion table on back fly-leaves.

Mass Spectra

Atlas of mass spectral data. E. Stenhagen, S. Abrahamson and F.W. McLafferty. New York: Interscience; 1969. 3 volumes.

Lists approx. 20,000 organic and inorganic compounds. Includes spectra. Formula index.

Compilation of mass spectral data. A. Cornu and R. Massot. London: Heyden in cooperation with Université de France; 1979. 2d edition. 2 volumes.

Lists 10,000 organic compounds. Does not include spectra. Formula index.

CRC handbook of mass spectra of drugs. Irving Sunshine, editor. Boca Raton, FL: CRC Press; 1981. 457 pages.

CI and EI data indexed alphabetically and by molecular weight; approx. 500 EI curves with an 8-peak index. Combined index to all tables by compound name.

Eight peak index of mass spectra; the eight most abundant ions in 66,720 mass spectra, indexed by molecular weight, elemental composition and most abundant ions. 3rd edition. Nottingham: the Mass Spectrometry Data Centre, the Royal Society of Chemistry; 1983. 3 volumes in 7.

Designed to find compounds that correspond to particular mass spectral data. Volume 1 (2 parts): Spectra in ascending molecular weight order, sub-ordered on number of carbon atoms, hydrogen atoms, etc. Volume 2 (2 parts): Spectra in ascending molecular weight order, sub-ordered on mass/charge values in order of decreasing abundance. Volume 3 (3 parts): Spectra in ascending mass/charge value order, where each mass/charge is the first and then the second most abundant, sub-ordered on the mass/charge values in order of decreasing abundance.

Handbook of static secondary ion mass spectrometry. D. Briggs, A. Brown and J.C. Vickerman. Chichester, NY: J. Wiley; 1989. 156 pages.

Section A discusses the principles of static SIMS. Section B provides reference spectra from a range of materials with attempted assignment of characteristic peaks. Section C provides more reference spectra and case studies of actual applications of SIMS.

Index and bibliography of mass spectrometry, 1963-1965. Fred W. McLafferty and John Pinzelik. New York: Interscience. 1 volume. Unpaged.

KWIC indexing.

Mass and abundance tables for use inn mass spectrometry. J.H. Benyon and S.E. Williams. Amsterdam: Elsevier; 1963. 570 pages.

Restricted to the four most common elements of organic chemistry (C,H,N,O); combinations restricted to those containing at least one atom of C and 6 or fewer of N or O, and H atoms not exceeding the number required to give a fully saturated molecule. All masses calculated relative to the mass standard $^{12}C = 12u$. Introduction in English, German, French and Russian.

Selected mass spectral data. American Petroleum Institute. Research Project 44. Washington, DC: American Petroleum Institute; 1947-. Looseleaf.

Principally hydrocarbons and compounds of interest to the petroleum industry. Standard and matrix formats. 2,259 standard spectra through 1975 and 432 matrix spectra through 1976. Indexed; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

Tables for use in high resolution mass spectrometry. Robert Binks, J.S. Littler and R.L. Cleaver. London: Heyden in cooperation with Sadtler Research Laboratories: 1970. 160 pages.

Tables devised to help the operator of a high resolution mass spectrometer to find the exact masses and hence the elemental composition . . . of any peak in mass spectrum by comparing it with a peak of known composition in the spectrum of a reference compound.—Introduction. Inserted (in pocket): "Chemical formulae from mass determinations."

The Wiley/NBS registry of mass spectral data. Fred W. McLafferty and Douglas B. Slauffer. New York: Wiley; 1989. 7 volumes.

Combination of the revisions of two books and their data base versions: *Registry of mass spectral data* (Stenhagen, Abrahamson and McLafferty) and *EPA/NIH mass spectra data base and its two supplements* (Heller & Milne). "[an attempt] to obtain the mass spectral data of as wide a variety of compounds as possible . . . this collection has been limited to unit-resolution mass spectra obtained by ionization at conventional electron energies (~70eV)"—Preface. Arranged by nominal molecular weight and Hill/CAS system.

Indexed by compound name, molecular formula, and CAS registry number.

Nuclear Magnetic Resonance Spectra

Aldrich library of NMR spectra. 2d edition. Charles Pouchert. Milwaukee: Aldrich Chemical Company: 1983. 2 volumes.

Consolidates the eleven volumes of the first edition with an additional 2,000 spectra; therefore provides spectra for more than 4,000 compounds. Molecular formula, alphabetical and Aldrich catalog number indexes at end of volume 2.

Formula index to NMR literature. M. Gertrude Howell, Andrew S. Kende and John S. Webb, editors. New York: Plenum; 1965. 2 volumes.

Lists approximately 8,300 organic compounds with references through 1962.

Handbook of high resolution multi-nuclear NMR. C. Brevard and P. Granger. New York: Wiley; 1981. 229 pages.

Fine tuning your NMR spectrometer. Provides 83 NMR fingerprints of nuclei, including spectra.

Handbook of NMR spectral parameters. W. Brugel. London: Heyden; 1979. 3 volumes.

"Tabulated high resolution chemical shifts and coupling constants for organic compounds according to spin system." Parameters of 7500 cmpds grouped by parent compound. "Rapid Search Index" is an alphabetical list of about 400 classes of organic compounds. Expanded and rearranged edition of the collection published in 1967, (viz.: W. Brugel, *Nuclear magnetic resonance spectra and chemical structure*).

Handbook of proton-NMR spectra and data. Ashai Research Center, Tokyo, supervised by Shinichi Sasaki. Tokyo and Orlando, FL: Academic, 1985-. 11 volumes.

Projected as an open-ended series of spectra and data. As of 1986 consists of 8000 compounds divided into 10 volumes with 800 entries each. Each volume is indexed independently by name, molec-

ular formula, substructure and chemical shift. There is also a cumulative index for volumes 1-10.

Handbook of tritium NMR spectroscopy and applications. E.A. Evans et al. Chichester, NY: Wiley; 1985. 249 pages.

Reviews all aspects of the development and applications of ^{3}H NMR spectroscopy over 15 years of its routine use. Designed as a comprehensive handbook of information, references and basic test for users of radioisotopes in life sciences research. Includes bibliography.

NMR band handbook. Herman A. Szymanski and Robert E. Yelin. New York: IFI/Plenum; 1968. 432 pages.

Lists 1200 organic compounds; 4800 shifts. Does not include spectra. Formula and shift indexes.

NMR data tables for organic compounds. Volume 1. Frank Bovey. New York: Wiley; 1967.

4,230 compounds. Does not include spectra. Formula index.

Nuclear magnetic resonance spectra. Philadelphia, PA: Sadtler Research Laboratories; 1966-. Looseleaf.

52,000 spectra by 1990. Indexed through the *Sadtler cumulated comprehensive indexes.*

Nuclear magnetic resonance spectra and chemical structure. Werner Brugel, compiler. New York: Academic; 1967-. 235 pages.

Table of NMR parameters of compounds the spectra of which have been analyzed. Organic compounds only. Does not include spectra. Alphabetical index. Volume 1 only; updating was intended but abundance of material resulted in completely new edition in 3 volumes, viz. *Handbook of NMR spectral parameters.*

Proton and carbon NMR spectra of polymers. Quang Tho Pham, Roger Petriaud and Hugues Waton. Chichester, NY: Wiley: 1983-84. 3 volumes.

Indexed by name within broad chemical classes.

The Sadtler guide to NMR spectra. William Walter Simons and M. Zanger. Philadelphia, PA: Sadtler Research Laboratories; 1972. 542 pages.

A systematic presentation of interpreted NMR spectra, arranged

by proton type . . . selected from the *Sadtler catalog of NMR spectra* either because they represent examples of characteristic absorbance patterns or because they are commonly encountered proton types. Indexed by spin system, coupling contents and exchangeable proton types as well as alphabetically.

The Sadtler guide to the NMR spectra of polymers. William Walter Simons and M. Zanger. Philadelphia, PA: Sadtler Research Laboratories; 1973. 298 pages.

Illustrates the spectra of a variety of common polymers and copolymers. Includes "Polymer Find Chart" and manufacturer, commercial name and alphabetical indexes.

Sadtler handbook of proton NMR spectra. William W. Simons, editor. Philadelphia, PA: Sadtler Research Laboratories; 1978. 1254 pages.

Arranged by functional group. Complementary to the handbooks of IR and UV spectra, containing the same compounds and using the same spectral numbering system. Alphabetical index; separate index volume also includes book order and chemical shift indexes.

Sadtler NMR spectra handbook of esters. Philadelphia, PA: Sadtler Research Laboratories; 1982. 686 and 159 pages.

The term 'esters' as used to describe the contents of this volume is applied only to the non-cyclic esters of carboxylic acids. Other types of esters will appear in future volumes dedicated to that group of compounds, e.g., sulfonic acid esters will be included with other compounds containing sulfur. 2,000 spectra selected from among those published in the Standard proton NMR collections between 1966 and 1980. Alphabetical, molecular weight and numerical indexes.

Selected nuclear magnetic resonance spectral data: 40 MHz, 60 MHz. American Petroleum Institute. Research Project 44. College Station, TX: Thermodynamics Research Center, Texas A & M; 1959-. Looseleaf.

Principally hydrocarbons and compounds of interest to the petroleum industry. 974 spectra by 1976. Index included in the 100 MHz collection; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

Selected nuclear magnetic resonance spectral data: 100 MHz. American Petroleum Institute. Research Project 44. College Station, TX: Thermodynamics Research Center, Texas A & M; 1974-. Looseleaf.

Principally hydrocarbons and compounds of interest to the petroleum industry. 414 spectra by 1976. Indexed; index includes 40, 60 MHz collection; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

100 MHz nuclear magnetic resonance spectra. Philadelphia, PA: Sadtler Research Laboratories; 1969-1970. 2 volumes. Looseleaf.

768 spectra. Indexed by name, chemical class and molecular formula.

Ultraviolet Spectra

Absorption spectra in the ultraviolet and visible region. L. Lang, editor. New York: Academic; 1961.

Lists approximately 6,000 organic and inorganic compounds. Includes spectra. Formula and substance indexes.

Atlas of protein spectra in the ultraviolet and visible regions. Donald Kirschenbaum, editor. New York: IFI/Plenum; 1972. 3 volumes.

Lists 1700 compounds. Includes spectra. Chemical substance index. Vol. 3: Bibliography of about 2500 citations for the 2434 indexed spectra.

Atomic and ionic spectrum lines below 2000 Angstroms: hydrogen through krypton. Raymond L. Kelly. American Chemical Society and the American Institute of Physics for the National Bureau of Standards; 1987. 3 volumes.

"Spectrum lines from the elements hydrogen through krypton, in all stages ionization, have been collected from the open literature and critically compared with the best values of atomic energy levels. The resulting list is ordered by element, spectrum number, and wavelength. The classification of each transition is given, along with the upper and lower energy level. A finding list [arranged by wavelength] is included." Issued as a supplement to the *Journal of Physical and Chemical Reference Data.*

Atomic spectra in the vacuum ultraviolet from 2250 to 1100 Å. Joseph Junkes, E.W. Salpeter and G. Milazzo. Citta del Vaticano: Specola Vaticano; 1965-.

Hollow cathode spectra. Chart of H_2 Lyman bands included.

Handbook of HeI photoelectron spectra of fundamental organic molecules: ionization energies, ab initio assignments, and valence electronic structure for 200 molecules. K. Kimura et al. Tokyo: Japan Scientific Societies Press and New York: Halsted; 1981.

Emphasis on substitution effects. Includes some simple inorganic molecules important as starting molecules for interpretation.

Handbook of ultraviolet and visible absorption spectra of organic compounds. Kenzo Hirayama. New York: Plenum; 1967. 642 pages.

Lists 8,443 compounds. Does not include spectra. No formula or substance indexes.

Organic electronic spectral data. New York: Interscience; 1946-.

Cooperative effort to abstract and publish in formula order all the UV-visible spectra of organic compounds presented in the journal literature from 1946 onward. Entries include solvent or phase and wavelength values. Organized according to molecular formula index system used by Chemical Abstracts. Does not include spectra. Large publication gap: volume 25, covering literature through 1983 was copyrighted 1989.

Sadtler handbook of ultraviolet spectra. Philadelphia, PA: Sadtler Research Laboratories; 1979.

Abridged edition of the Sadtler standard UV spectra collection intended as a small convenient collection of reference spectra of organic compounds relevant to introductory courses in organic chemistry, or as a desk reference when comprehensive collections are not available. Over 2,000 spectra representing the neutral, base and acid scans for 1600 compounds. Complementary to the handbooks of IR and NMR spectra, containing the same compounds and using the same spectral numbering system. Alphabetical, numerical and locater indexes.

Selected ultraviolet spectra data. American Petroleum Institute. Research Project 44. Washington, DC: American Petroleum Institute; 1945-.

Principally hydrocarbons and compounds of interest to the petroleum industry. 1178 spectra by 1976. Indexed; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

Ultraviolet spectra. Philadelphia, PA: Sadtler Research Laboratories; 1960-. Looseleaf.

41,829 spectra through 1989. Indexed through the *Sadtler cumulated comprehensive indexes.*

Ultraviolet and visible absorption spectra: index, 1930-1963. H.M. Hershenson. New York, London: Academic; 1966. 3 volumes.

Lists bibliographic references for spectra of 73,000 organic and inorganic compounds. Chemical substance index.

UV atlas of organic compounds (the DMS-UV atlas). London: Butterworths; 1966-71. 5 volumes.

Lists approximately 1,000 compounds. Includes spectra. Indexes.

Miscellaneous and Various Spectra

Assignments for vibrational spectra of seven hundred benzene derivatives. Gyorgy Varsanyi. New York: Wiley; 1974. 2 volumes.

700 compounds (IR and Raman spectra). Spectra in volume 2.

Atlas of electron spin resonance spectra. Ya. S. Lebedev et al. Akademiia nauk SSSR. Institut khimicheskoi fiziki. New York: Consultants Bureau; 1963-1964. 2 volumes.

Subtitle: Theoretically calculated multicomponent symmetrical spectra. Author translation from Russian original.

Atlas of near infrared spectra. Philadelphia, PA: Sadtler Research Laboratories; 1981. ~999 pages.

Collection of reference NIR spectra of 1,000 compounds selected on the basis of their demand by research scientists, their value for

NIR methods development and their general usefulness in industry. Alphabetical and molecular formula indexes.

Atlas of spectral data and physical constants for organic compounds. 2nd edition. Jeanette Grasselli and William Ritchey, editors. Cleveland: CRC Press; 1975. 6 volumes.

Lists 21,000 compounds. Does not include spectra. Indexes and bibliographies.

Comprehensive index of API 44-TRC selected data on thermodynamics and spectroscopy. College Station, TX: Texas A & M University. Thermodynamics Research Center; 1968, 1974.

Includes compound name and formula indexes to the American Petroleum Institute Research Project 44 collections or selected spectral data.

CRC handbook of EPR spectra from quinones and quinols. Jens A. Pedersen, editor. Boca Raton, FL: CRC Press: 1985. 382 pages.

Compilation of EPR data of numerous semiquinones and related radicals. Some spectra included as examples; most data presented in tabular form. Compound index and subject index.

Données spectroscopiques relatives aux molecules diatomiques: spectroscopic data relative to diatomic molecules. B. Rosen. Oxford, New York: Pergamon; 1970. 515 pages.

"Completely recast" updating of the 1951 edition. The tables mainly deal with electronic spectra located in the infrared, the visible and the ultraviolet.

Electronic absorption spectra of radical ions. Tadamasa Shida. Amsterdam and New York: Elsevier; 1988. 446 pages.

Charts for approximately 700 ions of spectra produced in gamma-irradiated frozen solutions. Indexed by name and by molecular formula.

Handbook of Auger electron spectroscopy. 2d edition. Lawrence E. Davis et al. Eden Prairie, MN: Physical Electronics Industries; 1976. 252 pages.

Includes 115 spectra arranged by atomic number, introductory chapters on method, and alphabetical index.

High resolution spectral atlas of nitrogen dioxide 559-597 nm. Kiyoji Uehara and H. Sasda. Berlin and New York: Springer-Verlag; 1985. 225 pages.

"The major part of the book consists of an atlas..of the absorption spectrum and the Stark modulation spectrum of NO_2 measured using a cw dye laser." — Preface. Chapter 4 is a list of the literature of spectroscopic studies of the NO_2 molecule published between 1978 and the beginning of 1984.

Inductively coupled plasma-atomic emission spectroscopy; an atlas of spectral information. R.K. Winge et al., editors. Amsterdam and New York: Elsevier; 1985. 584 pages.

Presents 232 wavelength scans of 70 elements and 973 prominent lines with associated detection limits for 72 elements. Each section is arranged by chemical symbol.

Line coincidence tables for inductively coupled plasma atomic emission spectrometry. P.W.J.M. Boumans. 2d edition. New York and Oxford: Pergamon; 1980. 2 volumes.

The tables concern spectral interferences emitted by free atoms or ions of the concomitants of the sample. The principal aim is to aid line selection in any type analysis. 896 analysis lines of 67 elements are listed. Arranged alphabetically by symbol.

Raman/IR atlas organischer Verbindugen//Raman/IR atlas of organic compounds. (DMS) Weiheim: Verlag Chemie; 1978. 2 volumes.

Raman and IR spectra, reproduced together on the same page in each case, for about 1,000 compounds. Divided into 15 main groups and 93 classes. Indexed alphabetically, by formula, and by substituent.

Selected Raman spectral data. American Petroleum Institute. Research Project 44. Washington, DC: American Petroleum Institute; 1948-. Unpaged.

Principally hydrocarbons and compounds of interest to the petroleum industry. 652 spectra by 1976. Indexed; also indexed by compound name and formula in the *Comprehensive index of API 44-TRC selected data.*

Spectral atlas of nitrogen dioxide, 5530 to 6480Å. Donald K. Hsu, David L. Monts and Richard N. Zare. New York: Academic; 1978. 632 pages.

Chapter 1 is a line atlas of high resolution absorption spectra presenting approximately 19,000 prominent lines; Chapter 2 is a collection of rotational analyses in the region from 5700 to 6800Å; and Chapter 3 is an annotated bibliography.

Spectral atlas of polycyclic aromatic compounds. W. Karcher et al., editors. Dordrech and Boston: D. Reidel; 1985. 818 pages.

Provides several types of spectra for each of 42 PAC pollutants. Additional data supplied for each compound include sources, distribution, and biological effect (e.g., carcinogenic activity). Arranged by mass number; indexed by compound name.

Spectral data of natural products. Kazutaka Yamaguchi. Amsterdam, New York: Elsevier; 1970.

Lists data for IR, UV, NMR, mass spectra, optical rotatory dispersion and circular dichroism values for 4,350 compounds. Occasionally includes spectra. Chemical substance index.

Spectroscopic data. 1975-76. J.E. Melzer and S.N. Suchard. New York: IFI/Plenum. 2 volumes in 3.

Collection of spectroscopic information dealing primarily with the electronic spectra of diatomic systems. Does not include spectra. Volume 1 parts 1-2: Heteronuclear diatomic molecules (restricted to molecules that, from thermodynamic reasoning, could be produced in an electronically excited state by a chemical reaction between a ground state atom and a ground state molecule). Volume 2: Homonuclear diatomic molecules.

Spectroscopic references to polyatomic molecules. V.N. Verma. New York: IFI/Plenum; 1980. 126 pages.

Bibliography of about 900 organic ring compounds; arranged in alphabetical order.

Tables for emission spectrographic analysis of rare earth elements. Ch. Kerekes. New York: Macmillan; 1964. Unpaged.

Analysis lines for each rare earth element (and scandium and yttrium) given in order of decreasing wave length. Arranged by chemical symbol.

Tables of spectral data for structure determination of organic compounds. 2d edition. New York and Berlin: Springer-Verlag; 1989. 1 volume, various paging.

For organic chemists involved in the identification of organic compounds or the elucidation of their structure. Arranged by type of spectra. Translated from the 3rd German edition. Includes tables for ^{13}C-NMR, ^{1}H-NMR, IR, mass, and UV/VIS, as well as a section of summaries arranged by structural elements and a section containing rules of practical importance.

Tables of spectral lines. Aleksandr Zaidel et al. New York: IFI/Plenum; 1970. 782 pages.

Part 1 contains spectral lines of 60 elements in order of decreasing wavelength. Part 2 gives spectral lines of 98 elements individually for each. Part 3 contains auxiliary reference material.

NOTES

1. Paramagnetic species are those containing atoms with unpaired electrons.
2. *Beilsteins Handbuch der organischen Chemie.* Heidelberg, Germany: Springer-Verlag; 1881-.
3. *Gmelins Handbuch der anorganischen Chemie.* Frankfort, Germany: Gmelin Institute; 1817-.

NEW REFERENCE WORKS IN SCIENCE AND TECHNOLOGY

Arleen N. Somerville, Editor

Reviewers for this issue are: Julie M. Hurd (JMD), University of Illinois at Chicago; Isabel Kaplan (IK), University of Rochester; Donna Lee (DL), University of Vermont; Diane J. Reiman (DJR), University of Rochester; Bruce Slutsky (BS), St. John's University; Arleen N. Somerville (ANS), University of Rochester; Jack W. Weigel (JWW), University of Michigan.

GENERAL SCIENCE

The almanac of science and technology, what's new and what's known. Edited by Richard Golob and Eric Brus. Boston: Harcourt Brace Jovanovich; 1990. 531 p. ISBN 0-15-600049-4.

This is not a review of the year's developments in science, nor is it an in-depth history of science. Rather, it is truly an almanac, an easily readable account of current topics in nine general areas: astronomy, biology, brain and behavior, chemistry, computers, earth sciences, environment, medicine, and physics. There is an index, but no references and no bibliographies for further reading. The copy under review is marked "uncorrected proof," which may account for the generally poor quality of illustrations and occasional editors' correction marks on some figure numbers. Despite these cosmetic flaws, this is an interesting book to read for general awareness of what's happening in science. Chapters are each approximately sixty pages and cover about six topics. While not recommended for research collections, this book could prove quite a handy addition to a public or community college library, or to the leisure reading room of a university library. (IK)

solve; history; preparation; synonyms; references to other major sources and spectra when easily available. Name, Registry no., and Colour Index no. indexes facilitate rapid access. Recommended for all collections serving scientists with a need for data about stains and dyes. (ANS)

MATHEMATICAL SCIENCES

Archives of data-processing history: a guide to major U.S. collections. Edited by James W. Cortada. New York, NY: Greenwood Press; 1990. 181 p. $45.00.

In the history of science and technology, the history of computing has only recently attracted scholars and publishers. This book is meant to serve as a quick guide to significant collections of primary sources in the United States. The editor acknowledges in his preface that many more collections are likely to become accessible in the next decade as institutions recognize the potential value of the materials. Twelve contributed articles describe the archival holdings of governmental units, universities, corporations, museums, and centers such as the Charles Babbage Institute for the History of Information Processing, a leader in archival activities. The editor completes the volume with a concise bibliographical essay on U.S. archival holdings. Clearly, sufficient raw materials await the examination of historians of data-processing, and this book enhances access to important resources. Highly recommended for research collections in computer science, and the history of science and technology. (DJR)

PHYSICAL SCIENCES

Comprehensive medicinal chemistry; the rational design, mechanistic study, and therapeutic application of chemical compounds. Chairman of the Editorial Board: Corwin Hansch; Joint Executive Editors: Peter G. Sammes and John B. Taylor. 6 vols. Oxford, New York: Pergamon; 1990. $1995.00. ISBN 0-08-0325-30-0 (set).

The structure, structure-activity relationships, synthesis and design, chemistry, reactions, and pharmacological activities of medicinal substances are discussed comprehensively. Extensive references throughout the text refer to original articles. In most volumes the information is organized by function of the compound. Volume 2, for example, covers enzymes that serve as agents acting in various functions, such as those acting on nucleic acids. This volume includes an extensive discussion of beta-lactam antibiotics. Volume 3 covers receptors, such as neurotransmitter and autocoid receptors. This section includes a fifty page discussion of dopamine, with 144 references. Volume 4 is devoted to drug design. A good summary of orphan drugs is one of the specific topics grouped together in volume 1. Each chapter is written by recognized experts. The subject index in volume 6 is detailed and extensive. The "Drug Compendium" in volume 6 provides very brief information for over 5500 medicinal substances: chemical structure, name, molecular formula, type of drug, and Chemical Abstracts Service Registry Number. There are references to the other 5 volumes, if

the substances are covered, and a couple key references. A Classification Index lists substances by pharmacological activity. Recommended for libraries serving medical, pharmacology, and synthetic organic chemistry researchers if funds permit. (ANS)

CRC handbook of ion-selective electrodes: selectivity coefficients. Yoshio Umezawa, Editor. Boca Raton: CRC Press; 1990. 848 p. $295.00. ISBN 0-8493 0546-2.

This handbook lists selectivity coefficients for over 1600 electrodes along with their electrode characteristics. The information is arranged alphabetically under four headings: inorganic anions, organic anions, organic cations, and inorganic cations. The data is extracted from articles published in major journals from 1966 through summer of 1988. Recommended for comprehensive analytical chemistry collections. (ANS)

Dictionary of Astronomical Names. By Adrian Room. London and New York, Routledge, 1988, 282 p. $27.50. ISBN 0-415-01298-8.

This compilation begins with a 27-page review of the history and principles of astronomical nomenclature. There follows a brief "astronomical glossary" which defines basic, general terms such as *asteroid* and *refractor.* The "dictionary" portion lists the proper names of several hundred selected individual astronomical objects—stars, minor planets, constellations, planets, planetary satellites, and lunar features—along with a few descriptive or historical lines about each. Appendix I provides a brief essay on lunar nomenclature and a selected list of the names of lunar craters with the full names, dates, nationalities, and professions of the individuals whose surnames were applied to the craters. Appendix II gives a bit of background information on minor planet nomenclature and a list of the first 1000 minor planets to be discovered (out of approximately 3000 that have been discovered and numbered). There are indications much of the data were derived from primary sources, some of which are more comprehensive than the present work. The author, evidently not a professional astronomer, is a prolific compiler of dictionaries on sundry other subjects. This book is a useful quick-reference tool which is likely to be useful particularly in libraries lacking a complete collection of more comprehensive publications. (JWW)

Dictionary of Drugs. J. Elks and C.R. Ganellin, Editors. 2 vols. London: Chapman and Hall; 1990. $1099.00. ISBN 0-412-27300-4 (set).

This two volume set serves as a definitive source of concise data about significant drugs. It succeeds very well. The format is similar to the well known *Dictionary of Organic Compounds (DOC).* Entries are arranged alphabetically by name. Entries include: common names, Chemical Abstracts names linked to relevant Collective Indexes, Chemical Abstracts Service Registry Number,

structure diagram, molecular formula, physical and chemical properties for the parent compound and biologically active derivatives, therapeutic uses, hazard information, and references to major journal articles, patents, and reference books for preparation, spectra, toxicity, and biological activity.

The *Dictionary* includes substances that have significant pharmacological interest, including new drugs. Some entries are based on information in the *DOC*, but are substantially updated. A comparison of the adriamycin entries verifies this. The brief three inch entry for adriamycin in the 1982 *DOC* is extended to twenty inches. This expanded entry includes data about fourteen biologically active derivatives and includes twenty-six literature references, compared to four in 1982. The second volume includes the following indexes: name, molecular formula, Chemical Abstracts Service Registry Number, type of compound, and structure. Headings in the Compound Type index are based on pharmacological activity (anticonvulsants, immunostimulants, antineoplastic agents) or by compound type (tetracycline antibiotics, sulfonamides). Recommended for academic, medical, public, and industrial libraries which serve researchers in synthetic organic, pharmacology, and medicine. (ANS)

Guidebook to organic synthesis. 2nd ed. By Raymond K. Mackie, David M. Smith, and R. Alan Aitken. New York: Longman Scientific & Technical; copublished with Wiley; 1990. 387 p. $34.95. ISBN 0-470-21568-2 (Wiley).

This *Guidebook* is intended for students who are beginning a serious study of organic synthesis. It is a valuable concise summary of major synthetic methodology. The information is organized by broad type of reaction, such as formation of carbon-carbon bonds, ring closure and opening, oxidation, protective groups, and specific reagents. New chapters were added for asymmetric synthesis and selenium reagents. While the entire text was updated, the chapters on silicon and phosphorus reagents were expanded substantially. Specific name reactions such as Diels-Alder and Reformatsky and reaction types such as cycloaddition can be located readily using the subject index. The six pages that summarize the Diels-Alder reaction is a concise description, largely through detailed reaction schemes, of the reaction mechanisms with examples of major synthetic applications. The bibliography of further reading leads readers to selected books and journal articles. An essential book for all college and university collections. (ANS)

Handbook of natural products data. Volume 1. Diterpenoid and steroidal alkaloids. By Atta-ur-Rahman. Amsterdam, Oxford, New York, Tokyo: Elsevier; 1990. 962 p. $353.75. ISBN 0-444-88173-5.

This volume is the first of a new series that will bring together from scattered journal sources spectral data on natural products. These complex molecules are of interest because they offer a readily available source of various structural features which may be tested for biological activity. The first series volume published covers the diterpenoid and steroidal alkaloids. Alkaloids are naturally

occurring bases found in plants. The diterpenoids are those compounds with the molecular formula $C_{20}H_{32}$; steroidal alkaloids are those containing the perhydrocyclopentenophenanthrene nucleus.

This work includes data for 971 compounds as reported in the literature through 1988. The compounds listed are arranged according to their structural types in order of increasing molecular weight. For each compound the author provides a structural diagram, molecular formula, molecular weight, melting point, and Chemical Abstracts Service Registry Number. The scientific name of the plant(s) in which the compound occurs are listed with references to the original literature. UV, IR, ^{1}H-NMR, and ^{13}C-NMR spectral data are listed in descending order of magnitude. Older names for compounds and spectra for simple derivatives are also reported. End-of-the-book indexes provide access to the data by compound name, molecular formula, molecular weight, plant source and compound-type. A decision to purchase this series represents a major commitment of resources, but for those research collections with strength in the area of natural products chemistry this work should prove to be a time-saving reference and a first place to search for spectral data on natural products. (JMH)

Handbook of Space Astronomy and Astrophysics. By Martin V. Zombeck. 2nd ed. Cambridge & New York, Cambridge University Press, 1990. 440 p. $75.00 (hardcover); $34.50 (paperback). ISBN 0-521-34550-2 (hardcover); ISBN 0-521-34787-4 (paperback).

Emphasizing equations, tabular data, and graphs of observational findings, this handbook contains very little verbal explanation. Besides an opening chapter of "general data" and a concluding chapter on astronomical catalogs, there are seventeen more specialized chapters on astronomical and astrophysical subfields plus auxiliary subjects such as mathematics and statistics. At the end of each chapter there is a very brief list of source publications. There are occasional places where the data are not as current as possible. For example it is disappointing that a book with a 1990 imprint date reproduces a table of natural satellites dating from 1983; hence, numerous satellites discovered by the Voyager spacecraft are not included. On the other hand there has been a substantial increase in the amount of material; the second edition contains 114 pages more than the first edition. Again, this is an assemblage of fairly standard information in a handy single-volume package and should prove to be a rather useful quick reference. (JWW)