# Finding Chemical Spectra and Spectral Data

## Online Sources

**Jump Down to Printed Sources**

### Beilstein Crossfire

This database of over 7 million organic compounds includes spectral data from the literature. Search for the compound by structure, name, registry number, or other data and check for spectral date in the Field Availability section of the compound record. These entries will often provide some basic details about the spectrum (peak, solvent), and a reference to the journal source.

### ChemExper Chemical Directory

CCD contains IR spectra (via interactive applet) for various compounds. The directory can be searched by registry number, molecular formula, chemical name or synonyms in different languages as well as by physical and chemical characteristics and combinations of those data. The CCD may also be searched by substructure. The data are submitted from various sources and should not be considered critically evaluated.

### Electromagetic Spectrum -- Diagrams

### NIST Atomic Spectra Database

The Atomic Spectra Database (ASD) contains data for radiative transitions and energy levels in atoms and atomic ions. Data are included for observed transitions of 99 elements and energy levels of 52 elements. ASD contains data on about 900 spectra from about 1 Angstroms) to 200 micrometers, with about 70,000 energy levels and 91,000 lines, 40,000 of which have transition probabilities listed. The most current NIST-evaluated data associated with each transition are integrated under a single listing. (NIST)

### NIST Chemistry WebBook

The WebBook contains IR spectra for over 8700 compounds, mass spectra for over 12,600 compounds, electronic / vibrational spectra for over 4100 compounds, UV/VIS spectra for 400 compounds, constants of diatomic molecules (spectroscopic data) for over 600 compounds, and ion energetics data for over 16,000 compounds, etc. (NIST)

### NIST Molecular Spectra Databases

Three databases of diatomic, triatomic, and hydrocarbon molecules were originally published as spectral tables in the Journal of Physical and Chemical Reference Data. Each covers primarily the microwave region with some data available for the radio frequency region. Rotational spectral lines for 121 diatomic molecules, 55 triatomic molecules, and 91 hydrocarbons have been tabulated. The isotopic molecular species, assigned quantum numbers, observed frequency, estimated measurement uncertainty, and reference are given for each transition.

**NMRShiftDB**

Web database for organic structures and their NMR spectra. It allows for spectrum prediction (currently only for carbon) as well as for searching spectra, structures and other properties. It features peer-reviewed submission of datasets by users. As of October 2004, the database contained about 11,000 structures and about 12,000 assigned spectra. Some browser compatibility issues; must have JavaScript and Java VM enabled.

**SciFinder Scholar (Chemical Abstracts)**

For post-1955 articles, it is best to start with a **CAS Registry Number**, then limit the retrieval to "Spectral Properties". For pre-1955 articles, it is better to use a freetext query in the Research Topic task area. Note: CAS indexing policy often ignores spectra or spectral data in an article unless that is the primary topic of the article. Spectral information reported incidentally or as part of the characterization of a synthesized compound will not be indicated in the CA record, and using the "spectral properties" limiter with the RN will miss it. In this regard, Beilstein is the more detailed indexing source, so it is important to check both when searching for organic spectra.

**SDBS Spectral Database**

Large database of chemical spectra, with thousands of IR, 1H-NMR, 13C-NMR, MS, and ESR spectra, searchable by name, formula, registry number. (National Institute of Materials and Chemical Research, Japan)

**Sigma-Aldrich Catalog**

FT-IR and NMR spectra of most compounds in the catalog are downloadable as PDF files. Search by catalog number, name, formula, CAS registry number. Chemical/physical information, structure image are displayable. Free registration is required.

**Spectra Online**

A searchable database containing over 6,000 IR, MS, NMR (proton, carbon and other nuclei), UV-VIS and NIR spectra. The database is a collection of public domain and other data contributed from various sources, including the EPA Vapor Phase FT-IR Library. Requires Javascript and Chime plugin. Free registration required to view spectra.

**X-Ray Photoelectron Spectroscopy Database**

The NIST X-ray Photoelectron Spectroscopy (XPS) Database gives easy access to the energies of many photoelectron and Auger-electron spectral lines. Resulting from a critical evaluation of the published literature, the database contains over 19,000 line positions, chemical shifts, doublet splittings, and energy separations of photoelectron and Auger-electron lines. A highly interactive program allows the user to search by element, line type, line energy, and many other variables. Users can easily identify unknown measured lines by matching to previous measurements. (NIST)

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## Selected Spectra Sources in Print

Jump to:

**General**
**Sadtler Spectra**
**IR**
**NMR**
**Mass**
**UV-VIS**
**Raman**
**Other**

Follow these steps as you begin your hunt for printed spectra:

1. For infrared (IR) or nuclear magnetic resonance (NMR) spectra of common organic compounds, start with the **Sigma/Aldrich spectra collections** in our Spectra Section (the thick black volumes on the desk). Spectra in these collections are arranged by functional group, which makes it easier to locate spectra of unknowns. Each set also has name and formula indexes. You can also use the **Aldrich Catalog** as a starting point: it notes the IR and NMR volume and page number for compounds that Aldrich sells.
2. For IR, proton-NMR, Carbon-13 NMR, or UV of organics, consult the **Sadtler Spectra Collections** shelved in the Spectra alcove (the green volumes). You must start with a known compound name or molecular formula, since the spectra are filed in random order.
3. For Mass Spectra (MS), consult the mass spectral printed collections listed **below**.
4. For other types of spectra, consult the smaller and specialized collections, indexes, and data books in the Spectra Collection, the most important of which are listed below.

This bibliography is primarily limited to collections of chemical spectra and spectral data, and reference works such as handbooks, encyclopedias, and dictionaries. It generally excludes textbooks, manuals, and theoretical discussions of spectroscopy.

Spectral collections listed on this page are marked with one or more of the following icons, indicating what type of compounds are included in them:

O --Organic Compounds
I --Inorganic/Metal Compounds
P --Polymers and Macromolecules
D --Drug Compounds
B --Biological Compounds

As a general rule of thumb, organic spectra are by far the most common in secondary collections. Spectra of inorganics, polymers, drugs, and biological substances are harder to find and often require an extensive literature search; certain types of spectra for these are rarely reported.

Titles marked with a ★ are particularly useful and recommended.

All titles listed are shelved in the **Chemistry Library Spectra section**, unless otherwise noted.

## GENERAL SOURCES

This section lists general reference works, as well as spectra collections that contain two or more different types of spectra.

**Acronyms and abbreviations in molecular spectroscopy: an enzyclopedic [sic] dictionary.**
QC 454 M6 W46 1990 (Springer, 1990)
Lengthy definitions, descriptions and applications of acronyms, abbreviations, and symbols used in all areas of spectroscopy, plus relevant literature citations.

**Atlas of spectral data and physical constants for organic compounds.**
QD 257.7 G7 1975 (6 vols., 2nd ed., CRC, 1975)
Tabular condensation of spectral data (IR, Raman, UV, 1H-NMR, 13C-NMR, MS) on 21,000 organic compounds, drawn from numerous published collections. Vol. 1 contains name/synonym directory, structures, and spectroscopic reference tables; vols. 2-4 contain the data tables; vols. 5-6 have indexes by molecular weight, melting and boiling point, WLN, and spectral data.

**Atomic spectra and atomic structure.**
QC 451 H453 1944 (2nd ed., Dover, 1944)
Classic treatise by Gerhard Herzberg.

**Dictionary of inorganic compounds.**
Handbook Table (5 vols., Chapman & Hall, 1992)
Substance entries in this multivolume handbook of inorganic/organometallic compounds list journal articles that contain spectral information. Indexed by name/synonym, formula, and registry number.

**Dictionary of organic compounds.**
Handbook Table (9 vols., 6th ed., Chapman & Hall, 1996)
Substance entries in this multivolume handbook of organic compounds list journal articles that contain spectral information. Indexed by name/synonym, formula, and registry number.

**Dictionary of spectroscopy.**
QC 450.3 D46 1982 (2nd ed., Wiley, 1982)
Brief explanations of terms most frequently used.

**Encyclopedia of spectroscopy.**
QC 450.3 P47 1995 (VCH, 1995)
General illustrated definitions of concepts and techniques.

**Encyclopedia of spectroscopy and spectrometry.**
QD 95 E55 2000 (3 vols., Academic Press, 2000)
3-volume set with articles on historical overview, theory, methods and instrumentation, and applications of all types of spectroscopy.

**Handbook of data on organic compounds. (HODOC)**
Handbook Table (7 vols., 3rd. ed., CRC, 1994)
Entries provide names, synonyms, structures, formulas (line and molecular), physical constants, and spectral data (IR, Raman, NMR, UV, Mass), as well as CAS registry numbers and Beilstein references. 3 volumes of indexes: vol. 7-- synonyms, vols. 8-9-- formula, mp, bp, mw, plus extensive spectral data indexes.

**Handbook of organic compounds.**

QC 462.85 W675 2001 (3 vols., Academic Press, 2001)
Compendium of methodology and information for organic materials, surfactants, and polymer spectra in the UV, visible, NIR, IR, and Raman regions. 2130 spectra in vols.2-3; alphabetical index in back of vol.1.

**Handbook of spectroscopy.**
QD 95 H27 (3 vols., CRC, 1974)
Tables of data and references of available data in various fields of spectroscopy. Each volume is indexed separately.

**Handbook of vibrational spectroscopy.**
QD 96 V53 H36 2002 (5 vols., Wiley, 2002)
Encyclopedic articles covering all aspects of infrared and Raman spectroscopy: theory, instrumentation, sampling techniques, sample characterization, data processing, and applications.

**Interpreting infrared, Raman, and nuclear magnetic resonance spectra.**
QD 95 N98 2001 (2 vols, Academic Press, 2001)
Text by R.A. Nyquist.

**Molecular spectra and molecular structure.**
QC 451 H463 1945 (4 vols., Van Nostrand, 1945)
Classic treatise by G. Herzberg. Vol. 1 = Spectra of diatomic molecules. Vol.2 = Infrared and raman spectra of polyatomic molecules. Vol. 3 = Electronic spectra and electronic structure of polyatomic molecules. Vol. 4 = Constants of diatomic molecules.

**Practical handbook of spectroscopy.**
QD 95 P73 1991 (CRC, 1991)
A condensation of the above Handbook of Spectroscopy, containing tables of reference data in the fields of x-ray, atomic, IR, Raman, and UV spectroscopic methods, as well as electron spin resonance, mass absorption coefficients, activation analysis, etc.

**Spectral data for PCBs.**
QC 463 B5 S65 1994 (Thermodynamics Research Center, 1994)
Mass and infrared spectra for all 209 polychlorinated biphenyls, with literature references. Registry number index, plus table of gas chromatography retention times.

**Spectral data for steroids.**
QC 463 S8 S64 1994 (Thermodynamics Research Center, 1994)
IR, UV, 1H and 13C NMR, and mass spectra for 211 steroids. Indexes by name, formula, and registry number.

**Spectrometric identification of organic compounds.**
QD 272 S6 S55 1998 (6th ed., Wiley, 1998)
Introductory chapters on mass, IR, 1H- and 13C-NMR spectroscopy, with problems and references. A popular basic text by Robert Silverstein.

**Spectroscopy source book.**
QD 95 S6368 1988 (McGraw Hill, 1988)
Handy one-volume abridgement of information from the McGraw-Hill Encyclopedia of Science and Technology (6th ed.). Covers origins, techniques, and other basics.

**Structure determination of organic compounds: tables of spectral data.**
QC 462.85 T313 2000 (3rd ed., Text + CDROM, Springer, 2000)
Compilation of spectral reference data for IR, UV-VIS, 1H and 13C NMR, and MS, with a guide to interpretation.

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## SADTLER SPECTRA COLLECTIONS

One of the largest cumulations of published chemical spectra, the Sadtler Standard Spectra series (the green volumes) are shelved in the Spectra alcove. Cumulative indexes to the Sadtler Standard Spectra sets are shelved together near the beginning of the Sadtler sets. Use these to locate spectra in the Sadtler sets held in the Chemistry Library: 13C NMR, IR Grating, IR Prism, Proton NMR, and UV.

The indexes are divided into three sections: Alphabetical, Molecular Formula, and Chemical Class, and also by date: the bound indexes cover spectra up to 1980, and the looseleaf supplements cover 1981-96. For best results try the Formula indexes first; Sadlter's nomenclature can be unpredictable. After locating your compound in the index, note the reference number from the appropriate column, and then consult the corresponding Sadtler set:

- Prism: Standared Infrared Prism [123 vols.]
- Grating: Standard Infrared Grating [123 vols.]
- UV: Standard Ultraviolet [170 vols.]
- NMR: Standard Proton NMR [118 vols.]
- C-13: Standard 13C NMR [210 vols.]

Other smaller Sadtler sets not indexed with the above include:

- Inorganics Standard IR Grating, 5 vols. with Index
- NMR: Standard Proton NMR (300MHz) 24 vols. with Indexes
- Standard Fluorescence Spectra, 8 vols. with Index
- Dyes, Stains, Pigments (UV), 6 vols. with Indexes
- DTA Thermograms (commercial substances), 7 vols. with Indexes

For more information about using the Sadtler collections, see the **Sadtler Spectra** page.

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## INFRARED SPECTRA

**Aldrich library of FT-IR spectra.**
QD 96 I5 P66 1997 (Desk) (3 vols., 2nd ed., Aldrich, 1997)
Condensed-phase IR spectra for over 18,000 compounds, arranged by chemical class and structural complexity. Indexed by name, formula, and CAS Registry Number.

**Aldrich library of infrared spectra.**

QD 96 I5 P67 1981 (Desk) (3rd ed., Aldrich, 1981)
12,000 IR spectra arranged in classes by order of increasing complexity. Indexed by name, formula and Aldrich catalog number.

**Analysis of surfactants : atlas of FT-IR spectra with interpretations.**
QC 463 S94 H8613 1996 (Hanser/Gardner, 1996)
IR spectra of anionic, cationic, amphoteric, and other types of surfactants. Indexes by trade name and name, pp.61-75. Generally known as "Hummel Spectra" after its author, D.O. Hummel.

**Atlas of near infrared spectra.**
QC 457 A77 1981 (Sadtler, 1981)
NIR spectra of 1000 selected organics. Indexed by name and molecular formula, in the Sadtler format.

**Atlas of plastics additives.**
TP 1142 H86 2002 (Springer, 2002)
772 FT-IR spectra; indexes by name and trade name.

**Atlas of spectral data and physical constants for organic compounds.**
see entry in GENERAL SOURCES section above.

**Coblentz Society desk book of infrared spectra.**
QC 457 C685 1980 (Coblentz Society, 1980)
1,700 IR grating spectra of common compounds. Indexed by name and formula.

**FT-NIR Atlas.**
QC 462.85 P47 1992 (VCH, 1993)
1,957 spectra in the wavenumber range 3800-10500 cm-1.

**Handbook of data on organic compounds. (HODOC)**
see entry in GENERAL SOURCES section above.

**Handbook of infrared and Raman spectra of inorganic compounds and organic salts.**
QC 457 N927 1997 (Academic Press, 1997)
4-volume set; indexes in front of vols. 2 and 3.

**Index of vibrational spectra of inorganic and organometallic compounds.**
QC 453 G74 1972 v.1 (CRC, 1972)
Fairly complete bibliography of IR and Raman spectra from the literature between 1935 and 1960, arranged by main element then by empirical formula. Entries provide line structural formula, state or solvent, spectrum type and wavenumber range, and literature reference.

**Infrared absorption spectra.**
QD 96 A2 H469 1959 (2 vols., Academic Press, 1959-64)
Index of IR spectra published in the journal literature, 1945-62. List of journals indexed in front of each volume.

**Infrared absorption spectra of steroids : an atlas.**
QC 463 S8 I5 (2 vols., Interscience, 1953-58)
Indexes by functional group and name in vol.2.

**Infrared and Raman characteristic group frequencies.** O I P B
QC 457 S69 2001 (3rd ed., Wiley, 2001)
Correlation charts and tables with sections on macromolecules, biomolecules, NIR, inorganics, minerals, glasses, etc.

**Infrared band handbook.** O I
QC 457 S983 1970 (2 vols., 2nd ed., IFI/Plenum, 1970)
Compounds arranged by wave number in cm-1, showing structural formula and literature reference. Empirical formula index in vol.2.

**Infrared spectra atlas of monomers and polymers.** P
QC 463 P5 I53 (Sadtler, 1980)
2000 spectra, arranged by chemical class and then in increasing order of complexity. With alphabetical index and Spec-finder. Common trade names and chemical names are both used.

**Infrared spectra of pesticides.** O
SB 960 V57 1993 (Dekker, 1993)
400 FT-IR spectra of commonly used pesticides and related metabolites. Entries include structure, CAS number, band maxima with relative intensities. Name and formula indexes.

**Infrared spectroscopy atlas for the coatings industry.** O P
TP 1140 C48 1991 (2 vols., 4th ed., Federation of Societies for Coatings Technology, 1991)
Contains 2,500 FT-IR spectra of polymers, resins, pigments, solvents, additives and other materials. Indexed by name, subject, and includes introductory text and a large bibliography.

**Inorganic library of FT IR spectra.** I
QC 457 I54 1998 (Nicodom, 1998)
Four-volume set from Nicolet. 1800 IR spectra of inorganic and relatated substances: v.1 - minerals; v.2 - boron compounds; v.3 - inorganics in KBr pellets; v.4 - inorganic analytical agents and commercial materials.

**Inorganics and related compounds.** I ★
QC 457 S35 5 vols. (Sadtler)
1300 IR absorption spectra of inorganic and coordination compounds. Alphabetical index in vol.5.

**Nicolet oil library of FT-IR spectra.** O
QD 96 I5 N536 1994-95 (Nicodom, 1994-95)
IR spectra of commercial oil products: fuels, grease, solvents. Indexes by name, origin, and type.

**NIR Polymer library of FT-IR spectra.** P
QD 96 I5 N577 1999 (Nicodom, 1999)
660 NIR spectra of polymers and related compounds.

**Pharmaceutical library of FT-IR spectra.** D
QD 96 I5 P537 1998 (Nicodom, 1998)
385 NIR (11,000-4,000 cm-1) spectra of samples commonly used in the pharmaceutical industry.

**Raman/infrared atlas of organic compounds.** O
QD 272 S6 S3713 1989 (2nd ed., VCH, 1989)

IR, far-infrared, and Raman spectra are given for 1044 compounds, with chemical name, structure, and conditions. Indexes by spectrum number, name, formula, and functional group/substituent.

**Rapra collection of infrared spectra of rubbers, plastics, and thermoplastic elastomers.**
QC 463 P5 S53 1997 (2nd ed., Rapra, 1997)
Transmission and pyrolysate (condensed phase) spectra of important rubber and plastics-based materials, including homopolymers, copolymers and blends, at 4cm-1 resolution, plotted in % transmission (4000-400 cm-1). Indexes by material type and trade name.

**Sadtler Infrared Spectra** -- **see above.**

**Sigma library of FT-IR spectra.**
QD 96 I5 K45 1986 (Desk) (2 vols., Sigma-Aldrich, 1986)
Over 10,000 spectra of important biochemicals, with name formula and CAS RN indexes in vol.2. Complements the Aldrich standard collections.

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## NMR SPECTRA

**Aldrich library of NMR spectra.**
QC 762 P69 1983 (Desk) (2 vols., Aldrich, 1983)
Contains over 37,000 spectra, with indexes by compound name, molecular formula, and Aldrich catalog number in the back of volume 2.

**Aldrich library of 13C and 1H FT-NMR spectra.**
QD 96 F68 P67 1993 (Desk) (3 vols., Aldrich, 1993)
12,000 compounds arranged by functionality; 13C peak tables are included with spectra. Indexes in vol. 3 by name, molecular formula, CAS registry number, and Aldrich catalog number.

**Atlas of carbon-13 NMR data.**
QC 462 C1 B73 (3 vols., Heyden, 1979)
NMR data compiled from published literature, with indexes of names, molecular formulas, class, molecular weights, chemical shifts.

**Atlas of spectral data and physical constants for organic compounds.**
see entry in GENERAL SOURCES section above.

**13-C NMR data for organometallic compounds.**
QC 454 N8 M315 (Academic Press, 1981)
Table of chemical shift data divided by nature of the ligand and then by metal. Scan the table of contents first to locate the correct region of the table.

**13-C NMR of natural products.**
QD 415 R214 1992 (2 vols., Plenum, 1992)
Vol.1: mono- and sesquiterpenes; vol.2: diterpenes. Compounds arranged by structural class, then by increasing molecular weight. Each volume has name, formula, mw, source, and compound-type indexes.

**Carbon-13 NMR spectra.**
QC 462 C4 J64 (Wiley Interscience, 1972)
Selected compounds representing a variety of carbon environments. Name, code, and shift indexes in front.

**CRC handbook of phosphorus-31 NMR data.**
QC 462 P1 H36 1991 (CRC, 1991)
Compilation of P-31 chemical shifts of organophosphorus compounds.

**Dictionary of concepts in NMR.**
QD 96 N8 H65 1992 (Clarendon Press, 1992)
Thorough definitions of NMR principles, jargon, and acronyms, with citations for further reading.

**Encyclopedia of nuclear magnetic resonance.**
Reference QC 762 E53 1996 (8 vols., Wiley, 1996)
General encyclopedia on all aspects and applications of NMR in physics, chemistry, materials science, geology, biology, and medicine.

**Handbook of data on organic compounds. (HODOC)**
see entry in GENERAL SOURCES section above.

**Handy and systematic catalog of NMR spectra.**
QC 762 A94 (University Science Books, 1980)
350 60MHz NMR spectra, with compound name and formula indexes.

**NMR spectra catalog.**
QC 762 V27 (2 vols., Varian, 1962-63)
700 spectra; each volume has name, functional group, and shift indexes.

**NMR spectra of polymers and polymer additives.**
QC 463 P5 B73 2000 (Dekker, 2000)
13C NMR spectra (with some 1H, 19F, 29Si, and 31P) of 300 polymers and additives.

**Proton and carbon NMR spectra of polymers.**
QC 463 P5 P76 2003 (5th ed., Wiley, 2003)
453 polymer spectra grouped in families and arranged alphabetically.

**Sadtler guide to carbon-13 NMR spectra of polymers.**
QC 762 S29 1988 (Sadtler, 1988)
353 spectra, arranged by compound type. Name and locator (peak) indexes.

**Sadtler guide to the NMR spectra of polymers.**
QD 139 P6 S52 (BioRad, 1973)
Small collection of NMR spectra of common polymers and copolymers. Indexes by name, commercial name, manufacturer, plus a "polymer finder" chart by chemical shift.

**Sadtler NMR spectra** -- **see above.**

**Solid-state NMR polymer spectra.**
QD 139 P6 S6 1990 v.1 (MRG Polymer Press, 1990)

13C, 15N, 29Si CP/MAS and solution spectra of various commercial polymers, textiles, and fibers.

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### MASS SPECTRA

**Atlas of spectral data and physical constants for organic compounds.**
see entry in GENERAL SOURCES section above.

**CRC Handbook of mass spectra of drugs.**
RS 189 C7 (CRC, 1981)
Tables and spectra. Main spectra section is arranged by base peak in ascending order; not otherwise indexed.

**CRC handbook of mass spectra of environmental contaminants.**
TD 193 H57 1992 (2nd ed., CRC, 1992)
533 common pollutants, indexed by name, CAS Registry Number, molecular weight, and spectral peaks.

**Eight peak index of mass spectra.**
QC 454 M3 E5 1991 (4th ed., RSC, 1991, 3 vols. in 7)
Eight most abundant ions in 81,000+ mass spectra, indexed by molecular weight, elemental composition, and mass-to charge ratio of the eight most abundant ions. Each entry also provides the relative intensities of the eight most abundant ions plus the parent ion, molecular formula, compound name, CAS registry number when available, and the code for the source spectrum.

**EPA/NIH mass spectral database.**
QC 100 U573, no.63 (4 vols, supplements, index; U.S. National Bureau of Standards, 1978-80)
Compiled by the NBS, this collection contains over 25,000 verified mass spectra in bar graph format, with CA index name, molecular formula, mol. wt., structural formula, and registry number. Arranged by increasing mol. wt. The index volume covers the set and its first supplement, by name, formula, mol. wt., and registry number. (Supplement 2 is on microfiche.) This set was later revised as and superseded by the *Wiley/NBS registry of mass spectral data* (see below).

**Handbook of data on organic compounds. (HODOC)**
see entry in GENERAL SOURCES section above.

**Index of mass spectral data.**
QC 454 M3 A47 1969 (ASTM, 1969)
Index of 8000 mass spectra from the ASTM Committee E-14. Data consist of six strongest peaks and their relative intensities. Indexes by molecular weight and the six descending peaks.

**Ion mass spectra.**
QC 454 M3 M54 (Wiley, 1974)
Tabulation of ion mass spectra for 100 elements and compounds ionized in a low-voltage ion source. Index of ions on pages 25-27.

**Mass spectral and GC data of drugs, poisons, pesticides, pollutants, and their metabolites.**

RS 189 P425 1992 (4 vols., 2nd ed., Wiley VCH, 1992-2000)
Over 6400 mass spectra.

**Mass spectrometry desk reference.**
QD 96 M3 S73 2000 (Global View, 2000)
Concise reference for newcomers and practitioners.

**Wiley/NBS registry of mass spectral data.**
QC 454 M3 M395 1989 (7 vols., 2nd ed., Wiley, 1989)
Spectra are arranged in order of increasing molecular weight, then by molecular formula. Indexes in vol. 7 for compound names, molecular formulas, and CAS registry numbers. No peak indexes. This set is a revision and expansion of the *NIH/EPA mass spectral database* published by the NBS 1978-80.

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## ULTRAVIOLET AND VISIBLE SPECTRA

Looking for **Molar Absorption Coefficients (ε)**?

**Absorption spectra in the ultraviolet and visible region.**
QC 437 A19 (Academic Press, 1961-82)
24 volumes, edited by L. Lang. Each has its own index, and there are also cumulative index volumes for 1-5, 6-10, 11-15, 16-20.

**Atlas of protein spectra in the ultraviolet and visible regions.**
QC 463 P7 K5 (2 vols., IFI/Plenum, 1972-74)
Indexes by name and source.

**Atlas of spectral data and physical constants for organic compounds.**
see entry in GENERAL SOURCES section above.

**Handbook of data on organic compounds. (HODOC)**
see entry in GENERAL SOURCES section above.

**Handbook of ultraviolet and visible absorption spectra of organic compounds.**
QD 291 H5 (Plenum, 1967)
Part 1 is a table of absorption maxima arranged by chemical structure of the chromophore. Part 2 is the same list arranged by absorption maxima.

**Organic electronic spectral data.**
QC 437 O65 (Wiley, 1946-89)
Annual index of UV-visible spectra of organic compounds published in the journal literature. Compounds are arranged in Hill formula order and show UV max and logε with a literature reference. A big drawback to this series is that there is no cumulative index; every volume must be consulted.

**Sadtler Ultraviolet Spectra** -- **see above.**

**Sigma-Aldrich handbook of stains, dyes and indicators.**
Reference QD 77 G73 1990 (Aldrich Chemical Co., 1990.)
Alphabetical handbook of 525 common stains and indicators, with lambda-max and UV spectra. Indexed by name/synonym, registry number, lambda-max, C.I. number.

**Tables of spectrophotometric absorption data of compounds used for the colorimetric determination of elements.**
QD 113 I55 (IUPAC/Butterworths, 1963.)
UV data on elements. Each entry contains: anion or cation formula, colorimetric reagent(s), formula of the colored complex, medium, absorption spectrum, extinction coefficient, Beer's Law range, experimental procedure, interferences, and references.

**TRC spectral data: ultraviolet.**
QC 459 A45 1945-84 (10 vols., Thermodynamics Research Center, 1945-84; 1985-99)
UV spectra from the Thermodynamics Research Center Hydrocarbon Project. Formula indexes in each vol. 5.

**Ultraviolet and visible absorption spectra.**
QC 437 U477 (3 vols., Academic Press, 1956-66)
Index of otherwise hard-to-find UV/visible spectra published in 27 major journals between 1930 and 1963. Nomenclature in the index is irregular; the odd journal abbreviations used are defined in the introduction. A * next to a reference indicates a UV spectrum 200-350 mμ (may also include visible portion); ** indicates a vacuum UV spectrum below 200 mμ (may also include UV-VIS regions); no asterisk indicates visible region, 350-800 mμ. Compiled by H.M. Hershenson.

**Ultraviolet spectra of aromatic compounds.**
QC 459 F7 (Wiley, 1951)
600 spectra, indexed by name and formula.

**UV-VIS atlas of organic compounds.**
QC 462.85 P47 1992 (2nd ed., VCH, 1992)
Name and formula and R-number indexes in vol.2. (This is a revision of the DMS *UV atlas of organic compounds* that was published in looseleaf from 1966-71.) Compiled by H.-H. Perkampus.

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### RAMAN SPECTRA

**Atlas of spectral data and physical constants for organic compounds.**
see entry in GENERAL SOURCES section above.

**Handbook of data on organic compounds. (HODOC)**
see entry in GENERAL SOURCES section above.

**Handbook of Fourier transform Raman and infrared spectra of polymers.**
QC 463 P5 K86 1998 (Elsevier, 1998)
Indexes by name, trade name, general formula, and registry number.

**Raman/infrared atlas of organic compounds.**
QD 272 S6 S3713 1989 (2nd ed., VCH, 1989)
IR, far-infrared, and Raman spectra are given for 1044 compounds, with chemical name, structure, and conditions. Indexes by spectrum number, name, formula, and functional group/substituent.

**Raman spectra of polymers.**
QC 462 P5 H45 1993 (Wiley, 1993)
Small collection of Raman spectra of major commercial and natural polymers.

**TRC spectral data: Raman.**
QC 454 R36 A45 1948-83 (3 vols.); 1986-99 (4 vols.)
Raman spectra from the Thermodynamics Research Center Hydrocarbon Project. Formula indexes in vol. 3 and vol. 4.

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## OTHER SPECTRA

**Electronic absorption spectra of radical ions.**
QD 471 S535 1988 (Elsevier, 1988)
Index by molecular formula.

**Handbook of fluorescence spectra of aromatic molecules.**
QC 463 H9 B4 1971 (2nd ed., Academic Press, 1971)
Fluorescence and absorption characteristics, with molar extinction coefficients, of 200 compounds. Name and formula indexes.

**Handbook of X-ray photoelectron spectroscopy.**
QD 96 E44 H35 1995 (Physical Electronics, 1995)
XPS (ESCA) spectra, strong line spectra, and excited Auger spectra for most of the elements and some of their compounds, plus plots and tables of energy shift data.

**High resolution XPS of organic polymers.**
QD 139 P6 B43 1992 (Wiley, 1992)
X-ray photoelectron spectra of 100 standard homopolymers.

**Inductively coupled plasma-atomic emission spectroscopy.**
QD 96 P62 I38 1985 (Elsevier, 1985)
Compilation of 232 ICP wavelength scans of 70 elements, each covering an 80nm spectral region.

**Optical emission lines of the elements.**
QC 454 A8 P39 2000 (Wiley, 2000)
Database of electric-dipole emission lines of 90 elements and ions.

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