

RESEARCH GUIDE

Spectra Sources

George Mason University Libraries

Locations: Fenwick Library (Fen.) and Johnson Center Library (JCL). Also, some of these sources are on Permanent Reserve (Perm. Res.) at the Johnson Center Library.

Background Information on Spectroscopy

Encyclopedia of Analytical Science Fen. Ref. QD 71.5 .E53 1995 (10 vols)

Encyclopedia of Spectroscopy Fen. Ref. QC 450.3 .P47 1995

Encyclopedia of Spectroscopy and Spectrometry Fen. Ref. QD 95 .E55 2000 (3 vols)

Practical Handbook of Spectroscopy Fen. Ref. QD 95 .P73 1991

IR (Infrared)

Note: For the Sadtler Total Spectra Indexes (the **Green Binders**), read from the “**Grating**” column.

Source	If you know...	Use...
<u>Sadtler Standard Spectra: Infrared Grating Spectra</u> Fen. Ref. QC 453 .S312 (26 vols)	Chemical name	<u>Standard Total Spectra: Alphabetical Index</u> Fen. Ref. QC 453 .S19 (4 vols)
	Chemical class/Functional groups	<u>Standard Total Spectra: Chemical Classes Index</u> Fen. Ref. QC 453 .S191 (2 vols)
	Molecular formula	<u>Standard Total Spectra: Molecular Formula Index</u> Fen. Ref. QC 453 .S192 (2 vols)
	Sadtler IR grating number	<u>Standard Total Spectra: Numerical index</u> QC 453 .S3121
	Location of absorption peaks	<u>Standard Total Spectra: Standard Grating Spec-Finder</u> QC 453 .S3122

Other IR Sources

Source	Arranged by...	Indexes...
<u>Aldrich Library of FT-IR Spectra</u> (3 vols) JCL Perm. Res. QC 457 .P87 1997	Chemical class/Functional groups	Chemical name, molecular formula, CAS number, & Aldrich catalog number
<u>Aldrich Library of Infrared Spectra</u> JCL Perm. Res. QD 96 .I5 P67 1981	Chemical class/Functional groups	Chemical name, molecular formula, CAS number, & Aldrich catalog number
<u>Atlas of Near Infrared Spectra</u> Fen. Stacks QC 457 .A77	Random	Chemical name, molecular formula
<u>Sadtler Handbook of Infrared Spectra</u> Fen. Ref. QC 453 .S73 1978b JCL Perm. Res. QC 453 .S73 1978b	Chemical class/Functional groups	Chemical name, molecular formula, and location of absorption peaks
<u>Sadtler Spectra: Abused Drugs: Infrared</u> Fen. Ref. QC 457 .S3 C6 (2 vols)	Sadtler "AD" IR number	Chemical name and location of absorption peaks (Indexes in front of vol. 1)
<u>Sadtler Spectra: Inorganic & Related Compounds: Infrared</u> Fen. Ref. QC 457 .S3 I6 (4 vols)	Sadtler "Y" IR number	Chemical name, molecular formula, and Sadtler "Y" IR number (Indexes in front of vol. 4)

NMR (Nuclear Magnetic Resonance)

Note: For the Sadtler Total Spectra Indexes (the **Green Binders**), read from the "NMR" column.

Source	If you know...	Use...
<u>Sadtler Standard Spectra: NMR Spectra</u> Fen. Ref. QC 453 .S315 (23 vols)	Chemical name	<u>Standard Total Spectra Alphabetical Index</u> Fen. Ref. QC 453 .S19 (4 vols)
	Functional groups	<u>Standard Total Spectra: Chemical Classes Index</u> Fen. Ref. QC 453 .S191 (2 vols)
	Molecular formula	<u>Standard Total Spectra: Molecular Formula Index</u> Fen. Ref. QC 453 .S192 (2 vols)
	Also... Chemical name, molecular formula, functional groups, or Sadtler number	<u>Sadtler Standard Spectra: NMR Spectra Index</u> Fen. Ref. QC 453 .S315 Index (2 vols)
	Chemical shift	<u>NMR Chemical Shift Index</u> Fen. Ref. QC 453 .S3151 (3 vols)

Other NMR Sources

Source	Arranged by...	Indexes...
<u>Aldrich Library of 13C & 1H FT NMR Spectra</u> (3 vols) JCL Perm. Res. QD 96 .F68 P67 1993	Chemical class/Functional groups	Chemical name, molecular formula, or CAS number
<u>Aldrich Library of NMR Spectra</u> (2 vols) JCL Perm. Res. QD 96 .N8 P68 1983	Chemical class/Functional groups	Chemical name, molecular formula, or CAS number
<u>Sadtler Guide to NMR Spectra</u> Fen. Ref. QC 490 .S5 S3	Chemical class/Functional groups	Chemical Name, chemical shift, and coupling constants
<u>Sadtler Handbook of Proton NMR Spectra</u> Fen. Ref. QC 762 .S3 1978 (2 vols)	Chemical class/Functional groups	Chemical name and chemical shift in a separate index: Fen. Ref. QC 762 .S3 1978 Index

UV (Ultraviolet)

Note: For the Sadtler Total Spectra Indexes (the **Green Binders**), read from the “**UV**” column.

Source	If you know...	Use...
<u>Stadtler Standard Spectra: Ultraviolet Spectra</u> Fen. Ref. QC 459 .S34 (20 vols)	Chemical name	<u>Standard Total Spectra Alphabetical Index</u> Fen. Ref. QC 453 .S19 (4 vols)
	Functional groups	<u>Standard Total Spectra: Chemical Classes Index</u> Fen. Ref. QC 453 .S191 (2 vols)
	Molecular formula	<u>Standard Total Spectra: Molecular Formula Index</u> Fen. Ref. QC 453 .S192 (2 vols)
	Sadtler UV number	<u>UV Numerical Index</u> Fen. Ref. QC 459 .S34 Index
	Location of absorption peaks	<u>UV Locator</u> Fen. Ref. QC 459 .S34 Locator

Source	Arranged by...	Indexes...
<u>UV-VIS Atlas of Organic Compounds</u> Fen. Folio QC 462.85 .P47 1992 (2 vols)	Chemical class or function	Chemical name, molecular formula, and R-number

MS (Mass Spectrometry)

Source	Arranged by...	Indexes...
<u>Wiley/NBS Registry of Mass Spectral Data</u> Fen. Ref. QC 454 .M3 M395 1989 (7 vols)	Molecular weight	Chemical name and molecular formula

Electronic Spectra Sources—These resources can only be found on a stand-alone computer station located in the reference room of Fenwick Library.

Sadtler Spectroscopy Suite (CD-ROM)

Consists of four programs (you will usually want to start with *IR SearchMaster* or *ChemWindow*):

ChemWindow—Primarily a chemistry and spectral publishing program. Publish 2-D and 3-D chemical structures, spectral data, chromatograms, and peak tables. After a structure is drawn, **ChemWindow** can be used for MS interpretation, IR correlations, and C-13 and H-1 NMR predictions. Can also draw laboratory setups and engineering processes. Items can be annotated and labeled.

IR Mentor—An analysis program that is a database of spectral information used to assist in the interpretation of infrared spectra, particularly in the condensed phase. Access over 700 interpretive frequencies of more than 200 functional groups from alkanes to azides. Can be used to correlate functional groups to IR peaks in unknown spectra.

IR SearchMaster—Search databases of IR spectral data, not only by individual spectra, but also by peaks, bands, chemical names, chemical structure (using **ChemWindow**), and physical properties. Can be used with **IR Mentor** to correlate peaks.

SymApps—A 3-D visualization program. Can be used to convert 2-D structures to 3-D.

Aldrich SpecID Plus (CD-ROM)—Condensed Phase and Vapor Phase

This is the electronic version of the Aldrich Library of FT-IR Spectra (see top of page 2). SpecID consists of 2 CD-ROMs. The first disc is a database of the IR spectra of over 10,600 unique compounds in the condensed phase (volumes 1-2 of the print version). The other disc is a database of the IR spectra of over 6,600 unique compounds in the vapor stage (volume 3 of the print version). Users can *only* search graphically by spectra.

Aldrich/ACD Library of FT-NMR Spectra Pro (CD-ROM)

This is the electronic version of the Aldrich Library of 13C & 1H FT NMR Spectra (see top of page 3). This resource gives access to high-resolution 300 MHz H-1 NMR and 75 MHz C-13 NMR spectra of over 11,800 organic compounds. It allows the user to search spectra according to chemical name, molecular formula, CAS number, Aldrich catalog number and book reference. This version offers the advantages of text searching by molecular weight, location of peaks/NMR chemical shifts, boiling point, melting point, flash point, refractive index, density, chemical category, and solvent. It allows the user to graphically search by spectra, subspectra, and structure using the ChemSketch program. In addition, it allows the user to print spectra, structures, and technical data.

Finding Chemical Synonyms:

Many chemicals are known by several different names. If a reference source does not mention a chemical, look under an alternate name. The following sources are useful for finding chemical synonyms:

Chemical Nomenclature Guides

Aldrich Catalog/Handbook of Fine Chemicals Fen. Ref. and JCL Perm. Res. TP 202 .A54

Chemical Abstracts Index Guide Fen. Index QD 1 .C5 (2 vols, blue)

Dictionary of Organic Compounds Fen. Ref. QD 246 .D5 1996 (10 vols) (name, molecular formula, and CAS registry # indexes); JCL Stacks QD 246. D5 1982 (7 vols + 4 supplements) (name, molecular formula, and CAS registry # indexes in vol. 6 and cumulative indexes in supplements)

Merck Index Fen. Ref. Desk, JCL Ref., and JCL Perm. Res. RS 51 .M4 1996

* Also, look in the QD 4 and QD 5 call number areas for additional chemical dictionaries and encyclopedias.

Systematic Nomenclature Guides

CRC Handbook of Chemistry and Physics Fen. Ref., JCL Ref., and JCL Perm. Res. QD 65 .H3 (newest edition at Fen. Ref. Desk)

A Guide to IUPAC Nomenclature of Organic Compounds Fen. Stacks QD 291 .I57 1993

Filing Rules in Chemical Reference Sources (Alphabetical Ordering)

Some sources split chemical names and invert the pieces so that the "parent compound" is listed first in the alphabetical filing. For example,

trichloromethane \longrightarrow methane, trichloro

Most sources file alphabetically, disregarding italicized terms, locants (numbers), and punctuation, unless the chemical names listed in succession are identical. For example:

3-Bromo-2-butanol
1-Bromo-2-butene
tert-Butylamine
1-Chlorobutane
2-Chlorobutane
8-Chloroethyl acetate
cis-5, 6-Dimethyl-1, 3-cyclohexadiene
trans-5, 6-Dimethyl-1, 3-cyclohexadiene
Propyl hydrogen sulfate
2,2,2-Trichloroethanol

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