

SOME INFORMATION SOURCES FOR SPECTRA OF COMMON COMPOUNDS

UNDERGRADUATES DOING VERIFICATION OF UNKNOWNNS, IF YOU ARE HAVING PROBLEMS FINDING YOUR COMPOUND IN THESE RESOURCES, *talk with a Reference Person*. IF YOUR COMPOUND IS NOT IN THESE RESOURCES, *talk to your T.A.*

<u>REFERENCE TOOL</u>	<u>SIZE/SCOPE</u>	<u>ARRANGEMENT OF COMPOUNDS</u>	<u>INDEXES, SPECIAL FEATURES</u>
(1) Aldrich Library of Infrared Spectra , 1981. (QD 96 I5 P87 1981) Physical Sciences REFERENCE	<ul style="list-style-type: none">• 1 volume• Presents 12,000 spectra giving large samples of each of the <u>important organic functional groups</u> (example: Aromatic Amides).	<ul style="list-style-type: none">• Sections are arranged by chemical class. Compounds are located based on their most complex functional group. [USE INDEXES.]	<ul style="list-style-type: none">• Alphabetical index• Molecular Formula index• Table of contents lists classes of compounds used.• Other indexes available.
(2) Aldrich Library of FT-IR Spectra , 1985-1989. (QD 96 I5 P874) Physical Sciences REFERENCE	<ul style="list-style-type: none">• 3 volumes, vol. 3 is index• Presents 11,000 spectra giving large samples of each of the <u>important organic functional groups</u> (example: Aromatic Ethers).	<ul style="list-style-type: none">• Sections are arranged by chemical class. Compounds are located based on their most complex functional group. [USE INDEXES.]	<ul style="list-style-type: none">• Cumulative Alphabetical index• Cumulative Molecular Formula index• Table of contents lists classes of compounds used.• Other indexes available.
(3) Sigma Library of FT-IR Spectra , 1986. (QD 96 I5 K29) Physical Sciences REFERENCE	<ul style="list-style-type: none">• 2 volumes (1986), vol. 2 is index• "The spectra...[for over 10,000 compounds]...<u>cut across the whole of biochemistry</u>...complimentary to the Aldrich Library of FT-IR Spectra".	<ul style="list-style-type: none">• Compounds are arranged alphabetically within broad biochemical classes such as Amino Acids, Polysaccharides. [USE INDEXES.]	<ul style="list-style-type: none">• Alphabetical index• Molecular Formula index• Table of contents lists classes of compounds used.• Other indexes available.
(4) Merck FT-IR Atlas , 1988. (QC 457 M55 1988) Physical Sciences REFERENCE	<ul style="list-style-type: none">• 1 volume• 3,000+ Fourier transform-IR spectra of pure substances from the Merck-Schuchard program [<u>"those substances which were available to us</u>].	<ul style="list-style-type: none">• Compounds are arranged by molecular formula. [USE INDEXES.]	<ul style="list-style-type: none">• Useful indexes include:<ul style="list-style-type: none">• Molecular Formula index• Compound Name index

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REFERENCE TOOL

(5) **Aldrich Library of NMR Spectra**, 1983.
(QD 96 N8 P87 1983)
Physical Sciences
REFERENCE

(6) **Aldrich Library of 13C and 1H FT NMR Spectra**, 1993.
(QD 96 N8 P875)
Physical Sciences
REFERENCE

(7) **Eight Peak Index of Mass Spectra**, 1991.
(QC 454 M3 M41 1991)
Physical Sciences
REFERENCE

SIZE/SCOPE

- 2 volumes, vol. 2 is index
- Covers 37,000+ compounds (representing every class commonly encountered by chemists) (example: Phenols).

- 3 volumes, vol. 3 is index
- Contains combined proton and 13C NMR spectra of nearly 12,000 compounds representing products in the Aldrich Catalog (example: Aromatic Ketones).

- 3 volumes; 7 parts
- Over 80,000 mass spectra covering 65,600 compounds and elements.

ARRANGEMENT OF COMPOUNDS

- Sections are arranged by chemical class. Compounds are located based on their most complex functional group. [USE INDEXES.]

- Combined spectra are arranged by chemical class. Compounds are located based on their most complex functional group. [USE INDEXES.]

- The 8 most abundant ions in 81,123 spectra arranged by:
 - Molecular weight subordered by number of C, H, ... atoms (v.1).
 - Molecular weight subordered by mass to charge ratio (v.2).
 - Ascending order of mass to charge ratio (v.3).

INDEXES, SPECIAL FEATURES

- Cumulative Alphabetical index
- Cumulative Molecular Formula index
- Table of contents lists classes of compounds used.
- Other indexes available.

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- Indexes not present and not needed due to the arrangement of compounds which effectively indexes by:
 - Molecular Weight
 - Element Composition

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