

Sources of Spectral Information for Chemistry

{a} The Aldrich library of ^{13}C and ^1H FT NMR spectra, 1993.

Chemistry, Reference Spectra QC462.85;+A44X;1993;(LC)

Spectra Graphs, ^{13}C peak values included in addition to graphs

NMR — ^{13}C & ^1H (300 Mhz)

~12,000 organic compounds

listing by chemical class

Indices: alphabetic compound name, molecular formula, CAS registry number, Aldrich Catalog number.

{b} The Aldrich library of FT-IR spectra, 1985.

Chemistry, Reference Spectra QD96;I5;+P66X;1985;(LC)

Spectra Graphs

FT-IR (fourier transform) — condensed phase and vapor phase (GC-IR)

~11,000 condensed phase graphs; 6767 vapor phase graphs

maximum of 9 peaks listed

mostly organic, some inorganic compounds

listing by chemical class

Indices: alphabetic compound name, molecular formula, CAS registry number, Aldrich Catalog number

{c} The Aldrich library of infrared spectra -- Ed. 3, 1981.

Chemistry, Reference Spectra QD96;I5; +P67;1981;(LC)

The Aldrich library of infrared spectra -- 2d ed., 1975.

Kline Science, Reference QC457;+A43;1975

Spectra Graphs

IR — most grating, some prism

~12,000 spectra

organic compounds, some deuterated organometallics, and polymers

listing by chemical class

Indices: alphabetic compound name, molecular formula, Aldrich Catalog number.

{d} The Aldrich library of NMR spectra -- Ed. 2, 1983.

Chemistry, Reference Spectra QD96;N8;+P68X;1983;(LC)

The Aldrich library of NMR spectra, <1974>

Kline Science, Reference QD96;N8;+P68;1974

Spectra Graphs

NMR (60 Mhz)

~37,000 organic compounds (2nd edition)

listing by chemical class

Indices: alphabetic compound name, molecular formula, Aldrich Catalog number

{e} An atlas of spectral interferences in ICP spectroscopy, 1980.

Kline Science QD96;A8;P37;1980

Data Values

ICP (inductively coupled plasma)

listing by alphabetic sequence of element symbols

a portion also listed by increasing wavelength

update to MIT tables

{f} Atomic and ionic spectrum lines below 2000 angstroms : hydrogen through krypton, c1987.

Kline Science QC453;+K45;1987

Data Values

Spectral lines "below 2000 Å"
elements: hydrogen - krypton
listing by atomic order of element
Index to increasing wavelength
References to original literature

{g} ¹³C-NMR of natural products, 1992.

Kline Science QD415;R214X;1992

Data Values

¹³C NMR

listing by structural type

Indices: compound name (listed preferentially as trivial names), molecular formula,
molecular weight, natural source (under genus, species), compound class

References to original literature

{h} ¹³C NMR data for organometallic compounds, 1981.

Kline Science QD411;M35;1981

Data Values

¹³C NMR

organometallic compounds

information from literature; errors there not corrected.

listing "by nature of the organic ligand and then by the metal"

References to original literature

{i} Characteristic Raman frequencies of organic compounds, <1974>

Kline Science QC462.85;D64;1974 Chemistry QC462.85;D64;(LC)

Data Values and 108 Spectra Graphs in Appendix

Raman

organic compounds

Indices: frequency, author, and compound name, and molecular formula

{j} Chemical shift ranges in carbon-13 NMR spectroscopy , 1982.

Kline Science QD96;N8;B74;1982

Data Peak Shift Values

¹³C NMR

240,000 chemical shift values for 100,000 different substructure codes

listing by HOSE (Hierarchically Ordered Spherical Description of Environment)

structure code

{k} The Coblenz Society desk book of infrared spectra -- 2nd ed., 1982, c1977.
Sterling Memorial QC457;+C687X;1982

The Coblenz Society desk book of infrared spectra, c1977.

Chemistry, Reference Spectra QC457;+C685;1977;(LC)

Spectra Graphs

870 (1st ed.) - 900 (2nd. ed.) spectra

Grating IR

mostly organic compounds, a few inorganics

listing by chemical class

Indices: empirical formula, alphabetical name

{l} Compilation of reported ^{19}F NMR chemical shifts, 1970.

Kline Science QC462;F5;D86;1970

Data Peak Shift Values

^{19}F NMR (CF ^{13}C reference)

6022 chemical shift values

compounds grouped by connections to Fluorine

Original literature referenced at end of work

{m} Comprehensive index of API 44-TRC selected data on thermodynamics and spectroscopy, 1968.

Chemistry, Reference Spectra QC311;+T49;1968;(LC)

Index to:

Selected Infrared Spectral Data

Selected Ultraviolet Spectral Data

Selected Raman Spectral Data

Selected Mass Spectral Data

Selected NMR Spectral Data

Indices: compound name, molecular formula

{n} CRC atlas of spectral data and physical constants for organic compounds. <1973>

Kline Science, Reference QD291;+C18;1973 Chemistry, Reference Spectra QD291;+G73;(LC)

Data Point Values

^1H NMR (some ^{19}F , ^{13}C , P, ^{11}B); IR; Mass; UV

"values characteristic of compound structure, not necessarily ... a complete representation of the original spectrum"

~8000 organic compounds

listing by IUPAC names (1957 rules) [same as CRC Handbook of Chemistry and Physics]

Indices: compound names and synonyms, physical constants, or spectral data

{o} Donnees spectroscopiques relatives aux molecules diatomiques [Spectroscopic data relative to diatomic molecules], 1970.

Chemistry QC453;+R68;(LC)

Data Point Values

IR; Vis; UV

Diatomic molecules mostly inorganic

listed alphabetically by molecular formula

References to original literature

{p} Eight peak index of mass spectra : the eight most abundant ions in 81,123 mass spectra, indexed by molecular weight, elemental composition and most abundant ions -- 4th ed., 1991.

Chemistry, Reference Spectra QC454;M3;+M37;1991

Data Values

Mass

81,134 spectra covering 65,600 organic and inorganic compounds

v.1 listing by molecular weight and number of carbon atoms

v.2 listing by molecular weight and m/z

v.3 listing by m/z and most abundant ion

{q} FT-NIR atlas,1993.

Chemistry, Reference Spectra QC454;F7;+B822;1993;(LC)

Spectra Graphs

NIR (Fourier Transform Near Infrared) 3,800 cm^{-1} — 10,500 cm^{-1} wavelengths

~1900 compounds

listing by molecular formula

Indices: alphabetic compound name and CAS registry numbers

{r} Handbook of HeI photoelectron spectra of fundamental organic molecules: ionization energies, ab initio assignments, and valence electronic structure for 200 molecules.

Kline Science QC462.5;H34;1981

Spectra Graphs

UV photoelectron

221 mostly organic compounds. "simple inorganic molecules such as H_2O , NH_3 , etc. are also included"

listing by compound class

Indices: compound name and molecular formula

{s} Handbook of spectroscopy, <1974-

Kline Science, Reference QD95;H27;1974

Data Values, a few Spectra Graphs

X-Ray Spectroscopy - elements

ESCA/Photoelectron Spectroscopy - inorganic and organic compounds

Flame Spectroscopy - inorganic and organic compounds

Atomic Spectroscopy - metals and other elements

Emission Spectroscopy - elements

InfraRed Spectroscopy - mostly information on correlations and solvents

Raman Spectroscopy - compound classes

UV Spectroscopy - organic compounds

Electron Spin Spectroscopy - ions

Mass Spectrometry - organic compounds

NMR Spectroscopy - organic compounds

Indices include compound names

References to original literature

{t} Handbook of ultraviolet and visible absorption spectra of organic compounds, 1967.

Kline Science QD291;+H57;1967

Data Values

UV-Vis

Organic compounds

Table I listing by "chromophores" (absorbing system)

Table II listing by wavelength

References to original literature

{u} Infrared spectra and characteristic frequencies $\sim 700\text{-}300\text{ cm}^{-1}$, 1968.

Kline Science QC457;B46;1968

Spectra Graphs

Data Point Values for inorganic compounds

IR (cesium bromide)

1566 graphs of organic and inorganic (mainly metal oxides) compounds listing by chemical class

Index of molecular formula

References to original literature

{v} Ion mass spectra, 1974.

Kline Science QC454;M3;+W54;1974

Spectra Graphs

Mass

~ 100 elements and compounds mostly inorganics

"actual experimental data"

Index of ions

{w} Line coincidence tables for inductively coupled plasma atomic emission spectrometry, 1980.

Kline Science QD96;P62;+B68;1980

Data Values

ICP;Ar-ICP

896 analysis lines covering 67 elements

listing by wavelength and by alphabetical element symbol

{x} Massachusetts Institute of Technology wavelength tables : with intensities in arc, spark, or discharge tube of more than 100,000 spectrum lines most strongly emitted by the atomic elements under normal conditions of excitation between $10,000\text{ \AA}$. and 2000 \AA ., arranged in order of decreasing wavelengths -- 1969 ed., [1969]-c1982.

Kline Science QC453;M3;1969 Engineering, Reference QC453;M37;1969

Data Values

191,000 spectral data lines

elements

v.1 listing by spectral lines (decreasing wavelength)

v.2 expanded listing by alphabetic element symbol

{y} Molecular photoelectron spectroscopy; a handbook of He 584 Å spectra, <1970>

Chemistry QC453;M65;(LC)

Spectra Graphs

MPS

mostly organics, some elements and inorganics

listing by chemical class

Index includes compound names

{z} Molecular spectra and molecular structure -- 2d ed., <1950>-(1991)

Engineering QC451;H47;1950 Kline Science QC451;H47;1950

Spectra Graphs

~155 spectra

MPS

mostly organics, some elements and inorganics

listing by chemical class

Index includes compound names

{A} Organic electronic spectral data. v. 1- 1946/52-

Chemistry (Shelved in journal sequence by title) QC454;A2;O73;(LC) v.1-v.25 Kline Science

QD241;O74 v.1-v.12

fragmentary Data Values (λ_{max} & ϵ)

UV; Vis

Compounds included in collection if original literature describes at least one band by λ_{max} (maximum wavelength) and ϵ (molar extinction coefficient)

listing by molecular formula only

{B} Raman/infrared atlas of organic compounds -- 2nd ed, 1989.

Chemistry, Reference Spectra QD272;S6;+S3713X;1989;(LC)

Spectra Graphs

~1000 organic compounds

IR, far-IR, and Raman

listing by structure-related number system

Indices: spectrum number, compound name (derivatives listed under parent skeleton), molecular formula, functional group and substituent.

{C} Raman spectra of hydrocarbons, 1980.

Chemistry QC463;H9;+S7313;1980A;(LC)

Data Peak Values

Raman

hydrocarbons only

listing by molecular formula

Index of compound names

{D} Registry of mass spectral data, 1974-

Kline Science QC454;M3;+S74

Spectra Peak Graphs

Mass

18806 compounds

listing primarily by nominal molecular weight

Index of molecular formula

{E} Sadtler infrared spectra, 1956-

Chemistry, Reference Spectra v.1(1)-v.34(35,000)

Spectra Graphs

IR

Indices: alphabetic compound name; molecular formula; chemical class; molecular weight; cross-reference to other Sadtler spectra by IR spectra number

Includes SpecFinder Index to micron bands in sequence for unknown identification.

{F} Sadtler nuclear magnetic resonance spectra, 1966-

Chemistry, Reference Spectra 570;+S23

Spectra Graphs

¹H NMR

growing collection

Indices: alphabetic compound name; molecular formula; chemical class; cross reference to other Sadtler spectra by NMR spectrum number; molecular weight; chemical shift by proton type, increasing magnitude, and spectrum number sequence.

{G} Sadtler ultraviolet spectra

Chemistry, Reference Spectra v.1(1)-v.58(14,518)

Spectra Graphs

UV

Indices: alphabetic compound name; molecular formula; chemical class; molecular weight; cross-reference to other Sadtler spectra by UV spectra number

Includes UV Spectra Locator to millimicron bands in sequence for unknown identification.

{H} Catalog of infrared spectral data (API 44), 1943-

Chemistry, Reference Spectra 570;A5

Catalog of mass spectral data (API 44), 1947-

Chemistry, Reference Spectra 570;A54

Catalog of selected Raman spectral data (API 44) <1948-55>

Chemistry, Reference Spectra 570;A53

Catalog of ultraviolet spectral data (API 44), 1945-

Chemistry, Reference Spectra 570;A52

Selected nuclear magnetic resonance spectral data (API 44), 1968.

Chemistry, Reference Spectra 574;+A55

Selected ¹³C nuclear magnetic resonance spectral data (API 44), 1974-

Chemistry, Reference Spectra 570;A56

Spectra Graphs

contributions from participating laboratories in the American Petroleum Institute Project 44.

Comprehensive Index is shelved at Chemistry, Reference Spectra QC311;+T49;1968;(LC)

{I} Spectral data of natural products, 1970.

Kline Science QD95;Y35;1970

Primarily Data Point Values; some Spectra Graphs

NMR, UV, IR & Mass

listing by structure type

Index of compound names

{J} Tables of spectral data for structure determination of organic compounds -- 2nd ed., 1989.

Kline Science, Reference QC462.85:T313;1989

Data Values

¹³C, ¹H NMR; IR; Mass; UV-Vis

listing by functional group and substituents for interpretation and extrapolation to structure determination

{K} Tabulation of infrared spectral data, 1977.

Chemistry QC457:D64;(LC) Kline Science QC457:D64;1977

Data Values; 60 Spectra Graphs of "common organic solvents & impurities"

IR

mostly organic compounds, some inorganics

listing by chemical class

References to original literature

{L} UV-VIS atlas of organic compounds -- 2nd ed., 1992.

Chemistry, Reference QC462.85:+P47X;1992;(LC)

Spectra Graphs and Data Values

UV-Vis

listing by chemical class

Indices: spectra number; table number; molecular formula; alphabetic compound name; ring number

	Entry Number
¹³ C NMR- - - - -	-a, g, j, n, H, J
¹⁹ F NMR - - - - -	- - - - - l, n
¹ H NMR - - - - -	- - - - - a, d, n, F, J
Atomic Spectroscopy- - - - -	- - - - - -s
Compound Name - - - - -	a-d, g, i, k, m-n, q-s, y-z, B-C, E-G, I, L
Data Values - - - - -	- a, e-j, l, n-p, s-u, w-x, A, C, I-L
Electron Spin Spectroscopy- - - - -	- - - - - -s
Elements- - - - -	- - - - - e-f, s, v-w-z
Emission Spectroscopy- - - - -	- - - - - -s
Far-IR Spectroscopy - - - - -	- - - - - B
Flame Spectroscopy - - - - -	- - - - - -s
Graphs - - - - -	- - - - - a-d, i, k, q-r, s, u-v, x-z, B, D-I, K-L
ICP Spectroscopy - - - - -	- - - - - - e, w
InfraRed Spectroscopy - - - - -	- - - - - b-c, k, m-o, q, s, u, E, H-K
Inorganic- - - - -	- - - - - b, k, o-p, r-s, u-v, y-z, K
Ions - - - - -	- - - - - - s, v
Mass Spectroscopy- - - - -	- - - - - m-n, p, s, v, D, H-J
Molecular Formula - - - - -	-a-d, g, i, k, m, o, q-r, u, w-x, A-G, L
Molecular Weight- - - - -	- - - - - g, p, D-G
Nuclear Magnetic Resonance Spectroscopy - - - - -	- - - - - -a, d, g, j, l-n, s, F, H-J
Organic - - - - -	- - - - - a-d, i, k, n, p, r-u, y-z, B-C, J-L
Organometallic- - - - -	- - - - - - c, h
Photoelectron Spectroscopy - - - - -	- - - - - -r, y-z
Raman Spectroscopy- - - - -	- - - - - i, m, s, B, C, H
Registry Number - - - - -	- - - - - - a, b, q
Spectra Graphs - - - - -	- - - - - a-d, i, k, q-r, s, u-v, x-z, B, D-I, K-L
UltraViolet Spectroscopy- - - - -	- - - - - -m-o, r-t, A, G-J, L
Visible Spectroscopy - - - - -	- - - - - -o, t, A, J, L
Wavelength frequency - - - - -	- - - - - e, i, t, w-x
X-Ray Spectroscopy - - - - -	- - - - - -s