



# Suggested resources for spectral identification and interpretation

Appendix 1

PJ Larkin





## Books: Spectral Interpretation Principles

- Larkin, P.J. *Infrared and Raman Spectroscopy. Principles and Spectral Interpretation*, second edition; Elsevier: Cambridge MA, 2018
- Mayo, W.M., Miller, F.A., Hannah, R.W. *Course Notes on the Interpretation of Infrared and Raman Spectra: Deducing Structures of Complex Molecules*, first edition; John Wiley & Sons: New York, 2004
- Nakamoto, K. *Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A: Theory and Applications in Inorganic Chemistry, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, fifth edition; John Wiley & Sons: New York, 1997
- Socrates, G. *Infrared Characteristic Group Frequencies*, second edition; John Wiley & Sons: New York, 1994
- Lin-Vien, D.; Colthup, N.B.; Fateley, W.G.; Grasselli, J.G. *Infrared and Raman Characteristic Frequencies of Organic Molecules*, Academic Press: San Diego, 1991
- Colthup, N.B.; Daly, L.H.; Wiberley, S.E. *Introduction to Infrared and Raman Spectroscopy*, third edition; Academic Press: New York, 1990
- Bellamy, L.J.; *The Infrared Spectra of Complex Molecules, Vol 1*, third edition; Chapman and Hall: New York, 1975





## Books: Collections of Infrared Reference Spectra

- Aldrich Library of FT-IR Spectra, 3 Volume Set, Eds. Pouchert, C.
- Infrared Spectra of Inorganic Compounds (3800-45  $\text{cm}^{-1}$ ) Nyquist, R.A., Kagel, R.O.
- Atlas of IR Spectra of Organophosphorus Compounds (Interpreted Spectrograms), Shagidullin, R.R., Chernova, A.V., Vinogradova, V.S., Mkhametov, F.S., Springer, 1990
- Sprouse Collection of Infrared Spectra-Book 1 Polymers, J.F. Sprouse, D.L. Hansen, Sprouse Scientific Systems, Inc, 1987
- Atlas of polymer and plastics analysis, vol. 1, polymers: Structure and spectra, 2nd ed., D. O. Hummel ed., Carl Hanser Verlag, Munich, Germany 1978
- Analysis of Surfactants: Atlas of FTIR Spectra with Interpretations, Hummel, D.O., Baum, A., Oastura, A., Weber, A., 1996
- Raman/Infrared Atlas of Organic Compounds, Second Edition, B. Schrader, VCH
- The Coblenz Society Spectral Collections (5 volumes) see <http://www.coblentz.org/education/spectral-databases>
- An infrared spectroscopy atlas for the Coatings Industry, D. G. Anderson, S. K. Duffer, J. M. Julian, R. W. Scott, T. M. Sutliff, M. J. Vaickus, and J. T. Vandenberg, Federation of Societies for Coatings Technology, Philadelphia, 1980



---

## Training: IR (& Raman) interpretation course

- IR and Raman Courses at Bowdoin College (ME) <https://ircourses.org/> see Coblentz society



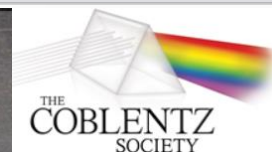
## Digital Libraries

### Free

- Spectral Database for Organic Compounds SDBS from National Institute of Advanced Industrial Science and Technology (AIST) Japan
  - [https://sdb.sdb.aist.go.jp/sdb/cgi-bin/cre\\_index.cgi](https://sdb.sdb.aist.go.jp/sdb/cgi-bin/cre_index.cgi)
- RRUFF project website for minerals
  - <https://ruff-2.geo.arizona.edu/>
- NIST Chemistry WebBook
  - <https://webbook.nist.gov/>

### Commercial

- Wiley Spectral Libraries (formerly Sadtler Spectral Libraries)
  - <https://sciencesolutions.wiley.com/solutions/technique/ir/>
  - ThermoFisher Scientific
    - <https://www.thermofisher.com/search/browse/category/us/en/602583/Spectral+Libraries>
- S.T. Japan-USA
  - [http://www.stjapan-usa.com/Products/SpectraDatabases/tabid/165/Default.aspx#ATR-FTIR\\_Spectra\\_Libraries](http://www.stjapan-usa.com/Products/SpectraDatabases/tabid/165/Default.aspx#ATR-FTIR_Spectra_Libraries)
- FDM (Fiveash Data Management, Inc)
  - <https://www.fdmspectra.com/index.html>
- The Coblenz Society Infrared Spectra Collections for ACD/Labs
  - <http://www.coblentz.org/education/spectral-databases>



## Commercial Software

### Selected Spectral Search Software

- KnowItAll (Wiley formerly BioRad) Software
  - <https://sciencesolutions.wiley.com/software/>
  - ACD/Labs Optical Spectroscopy software
    - <https://www.acdlabs.com/products/adh/uvir/>
- Peaks FTIR Spectroscopy Software
  - <https://www.peakspectroscopy.com/>
- FDM SearchFaster
  - [https://www.fdmspectra.com/FDM\\_SearchFaster\\_for\\_FTIR\\_and\\_Raman.html](https://www.fdmspectra.com/FDM_SearchFaster_for_FTIR_and_Raman.html)
- ❖ Note: Instrument vendor software (PE, Bruker, Thermo, Agilent) also includes spectral searching and data analysis functions

### Functional Group Analysis Software

- KnowItAll (Wiley formerly BioRad) functional group analysis
  - <https://sciencesolutions.wiley.com/knowitall-software-vibrational-spectroscopy-edition/>
  - irANalyze, LabCognition
    - <https://www.chemeurope.com/en/software/52403/ir-spectra-interpretation-iranalyze.html>



# Membership in Professional Societies Provide You So Many Dividends:



<https://www.s-a-s.org/>

Society for Applied Spectroscopy

- to advance and disseminate knowledge and information concerning the art and science of spectroscopy and other allied sciences
- publishers of the internationally recognized, peer reviewed journal **Applied Spectroscopy**.

<http://www.coblentz.org>

The Coblentz Society

- to foster the understanding and application of vibrational spectroscopy
- a technical affiliate of the [Society for Applied Spectroscopy](https://www.s-a-s.org/) (SAS)

