1) I have been a librarian for 2 years at the University of Rochester and I have inherited an excellent collection. I want to keep it up to date, so I volunteered to speak about spectroscopy to enhance my understanding of the subject and learn about new resources.
1) Today I want to pass on my learnings. Hopefully there will be something for everyone. I will provide some definitions especially for those new to this subject, I will discuss a few common techniques, and I will talk about resources that you may have for your library. My handout covers vendors and their contact information for the resources I will be discussing.
What is spectroscopy?

A method used to identify and/or quantify elements, atoms, molecules, matter, molecular structure by observing absorption, emission or scattering interactions with electromagnetic radiation ("light")

1) So what is spectroscopy? This is my definition derived from several sources, mainly Hawley’s Condensed Chemical Dictionary. SLIDE I had to laugh at one web site that I discovered on the history of spectroscopy. The first event was God Said “let there be light”.
1) But light is really the core of spectroscopy. Hard to describe what it is – but if you can see, you know it is there. Scientists call it electromagnetic radiation, and have described it as waves with electric and magnetic components. They include not only visible light, but slow & wide radio waves and fast and narrow gamma rays.
Electromagnetic Radiation

Equation: \( C = v \times \lambda \)

- Speed of light, \( C = 3 \times 10^{10} \text{ cm/sec} \)
- Frequency, \( v = \text{cycles per second in Hz} \)
- Wavelength, \( \lambda = \text{distance between adjacent wave crests in cm} \)
- Wave number, \( W = \text{inverse of Wavelength in cm}^{-1} \)

1) They use the length of a wave, or wavelength, and cycles per second, or frequency to identify types of light. Frequency and wavelength are related because no matter what type you are talking about, it travels at the same speed, \( C \), the speed of light.
1) In spectroscopy, light interacts with samples in three ways:

   Absorption. Light goes into the sample, but doesn’t come out.
   Emission. Light is given off.
   and Scattering. Light goes through the sample, but is changed and comes out at a different path and often a different frequency.
1) A spectrum is a graphical representation of how the sample and the light are interacting. Here is an Infrared Absorption spectrum. It shows wavenumbers, which are 1/wavelength v. Transmittance, which is related to absorbance. Chemists learn information about the structure of a compound by interpreting the spectra because each compound has a unique spectra, sort of like a fingerprint.
1) There are so many techniques in spectroscopy, that I could spend the whole afternoon telling you about them. I have chosen 5 common ones, Mass spectrometry, Raman Spectroscopy, Ultra Violet/Visible Spectroscopy, Infrared Spectroscopy, and Nuclear Magnetic Resonance Spectroscopy. The date beside them gives you an idea of when these techniques came into acceptance. Generally the data that you might find prior to the 40s and 50s will be of questionable quality. Because of many advancements in techniques in the 60s and 70s the best data can be found in the last 30 years.
1) Mass Spectrometry is not a spectroscopy technique, but I am telling you about it because Mass spec spectra are often bundled with other spectra in the resources. Mass Spectrometry involves the SLIDE
Raman Spectroscopy

Scattering of Infrared light due to molecular bond vibrations.

Key Parameters:
- peak location
- peak shape
- peak strength
- wave numbers
- transmittance

1) Raman Spectroscopy involves SLIDE
Ultraviolet/ Visible Spectroscopy (UV/Vis)

Absorption of Ultraviolet and Visible light due to electrons moving to higher energy levels

Key Parameters:
- molar absorptivity ($\varepsilon$)
- extinction coefficient
- maximum absorption ($\lambda_{\text{max}}$)
- absorbance

1) Ultraviolet/ Visible Light Spectroscopy, often call absorption spectroscopy, involves SLIDE
Infrared Spectroscopy (IR)

Absorption of Infrared light due to molecular bond vibrations.

Key Parameters:
- peak location
- peak shape
- peak strength
- wave numbers
- transmittance

1) Infrared Spectroscopy, often used by students in organic lab, involves...
Absorption of radio waves in the presence of a strong magnetic field used to determine molecular structure.

Nucleus types: H, C, F, P, N

Key Parameters:
- chemical shift: $\delta$ (delta), Tau
- frequency: ppm or hz
- coupling constant
- integrals

1) NMR is an extremely popular and well developed technique. It involves SLIDE Two dimensional NMR, COSY, HETCOR and NOESY spectra have achieved acceptance within the last 15 years.
1) Switching subjects here, much information has been recorded about spectroscopy. A primary source is articles so I will tell you how to find them. Data from experiments has been recorded in handbooks and spectra libraries. In fact, there has been a huge effort to record spectra systematically. Special software for capturing, comparing, manipulating, and reporting spectra has been developed. The accuracy and ease of spectra prediction is improving. Lastly, I want to share selected resources useful for learning: encyclopedias, text books and web sites.
1) Much of spectroscopy information is recorded in graphical form, a spectra. This is the format that is used in spectral libraries, sometimes articles. However, most articles contain spectral info in text or table form – very cryptic unless you know the code. In this example, the author from the J. Org. Chem article is talking about proton NMR, the solvent is CDCl₃, the shift, delta = 3.24, the peak is a singlet and represents 3 hydrogens in the CH₃N part of the molecule.
How to find spectroscopy articles

- Chemical Abstracts
- Beilstein/ Gmelin
- Special Indices

Chemical Abstracts, Beilstein, and Gmelin via Crossfire and some other indices are wonderful tools for finding articles.
Spectra info in Chemical Abstracts

- Search for chemical substance, then limit references to spectral properties (1967+).
  - In Scifinder Scholar, analyze by index term

- Older data (pre-1967) do a topic search on substance name and refine by technique and by range of years

- To enhance STN searches use the STN Lexicon to determine appropriate vocabulary
  - =>e spectroscopy+kt/ct
Here is the Scifinder Scholar screen that allows you to limit substance references to spectral properties.
Spectra Info in Beilstein/ Gmelin

- Look up substance of interest and use “field availability” to navigate to spectra references.
- Use the easy data search (EDS) screen for spectroscopy.
- Combine EDS search with structure or fact editor searches.

In Beilstein or Gmelin -- SLIDE
Here is the Field Availability screen in Beilstein. Depending on what compound you are looking at, you can get references to articles about various spectroscopy techniques by double clicking on your choice.
Here is the Easy Data Search screen in Beilstein – Gmelin has a similar one.
Sometimes you can get false hits when using Chemical Abstracts. When you look up compounds in the Combined Chemical Dictionary, you get references to NMR and IR spectra too, and these tend to be right on. This is the case with the whole set of books that Chapman and Hall have put out that start with “Dictionary of . . .” (Organic, or Organometallic for example). Often they have references to Aldrich’s spectral libraries. If you are looking for older spectra, IR or NMR, I have found Hershenson’s books to be useful.
Handbooks with Spectral Data

- Chapman & Hall/CRC's Properties of Organic Compounds

If you want to get your hands on NMR or IR data right away for common organic compounds, Properties of Organic Compounds and the Handbook of Data on Organic Compounds are very useful.
Sometimes textual data is not enough. Students especially want to visualize what is happening. Researchers want to manipulate, store or predict spectra. Here are several prominent databases and software. These are available electronically.

<table>
<thead>
<tr>
<th>Major Spectra Libraries &amp; Software</th>
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<tbody>
<tr>
<td>SDBS: Integrated Spectral Data Base</td>
</tr>
<tr>
<td>Sigma-Aldrich</td>
</tr>
<tr>
<td>ACD Lab</td>
</tr>
<tr>
<td>NIST Web Book</td>
</tr>
<tr>
<td>BioRad’s – KnowitAll™ / HaveitAll™</td>
</tr>
<tr>
<td>Wiley Chemical Concepts - SpecInfo</td>
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</table>
SDBS is on the web. It is a medium sized collection of IR, MS, NMR, Raman, and ESR spectra. There are several ways to search SLIDE. I really like the proton identification – correlating the spectrum with the structure. Most spectra are measured SLIDE. It is free within their guidelines. Notify them if you will be doing many downloads or they will block your access.
I have these Aldrich books in my library. They contain a small number of commonly used compounds. My students use them so heavily that we need to rebind them every year.
I find this CD of NMR spectra very exciting. Even though CD-ROMs are old technology, the searching is a great enhancement over the books. You can search by melting point, boiling point, as well as compound name, molecular formula and CAS Registry number. SLIDE If installed on a computer with internet access, you can link directly to the Sigma Aldrich web site …
where there is free access to IR spectra. By itself, the web site is a gem because there is free access to other physical properties, MSDS sheets and structures.
ACD’s version of Sigma-Aldrich FT-NMR

Software on CD with structure/ substructure searching sold separately or as plugin to Spec Manager

ACD Labs now provides a version of Aldrich’s C13/ FT-NMR collection that is structure searchable. If you like, you can get it as a plugin to their Spec Manager.
ACD’s Spec Manager

- Software (CD) for processing multiple spectra techniques (NMR, MS, UV-Vis, IR, Raman, GC, HPLC)
- Take raw data from spectrometer, process and store with experimental parameters.
- Search by: structure, substructure, shift, name of compound, user defined fields
- May assign structures using ChemSketch and correlate with spectrum peaks
- Single technique modules available: HNMR, UV-IR, MS, 2D-NMR Managers

Available on CD, Spec Manager can be used to process multiple types of spectra. Raw data can be imported into software right from an instrument. The user can add structures and whatever additional information they choose. They can then search by SLIDE.
ACD is well known for predicted physical properties many listed now in Chemical Abstracts. They also have software for predicting NMR spectra – for proton, C13, F, and N. This product could be especially useful to students who are learning spectra interpretation or researchers who are making new compounds.
If you like, you can add on a database of structures. These will lead you to the original references with experimental data. They can be searched in traditional ways.
Bio-Rad’s KnowItAll™

- Modular/ customizable software on CD. Various application options, such as Database Building, available at low cost.
- 4 Editions: Analytical, ChemWindow, Forensic, Student
- Features: Spectra retrieval, manipulation, prediction, interpretation, storage, reports, structure drawing, compound naming
- Search by: spectrum, peaks, compound name, CAS #, MF, MW, structure, substructure, physical properties, chemical properties . . .
- Review in JACS V. 124 (7) 2002 p. 1555

I have sets of green Sadtler binders in my library. The newest version of Sadtler information can be found using BioRad’s KnowItAll and HaveItAll products. KnowItAll is the software component on CD. SLIDE It can be used to build an in-house spectra library. It may be purchased for a one time fee.
BioRad’s HaveItAll™

- >500,000 high quality reference spectra on CD
- 4 major spectra sets
  - NMR: ~12,000 HNMR & ~147,000 CNMR
  - IR: ~230,000 IR & ~3,800 NEAR IR,
  - Raman: ~3,300
  - MS: ~107,000 (NIST)
- Includes structures and experimental conditions
- Can build collections for multiple techniques such as UV/VIS, GC, IR, 13C NMR, H NMR, Raman, NIR, MS
- Easy to move between techniques
- Databases available by subscription

HaveItAll is the database portion of BioRad’s offering. They have a very large, high quality spectra collection which includes SLIDE. If you are looking at the data for one compound, it is easy to bring up all the available information, including spectra generated using various techniques.
The NIST Web book is another free web resource. It contains a small collection of Spectra. There are many ways to search, including SLIDE.
Another major player in spectra software and libraries is Chemical Concepts, a Wiley company. They have 3 products SLIDE.
Spec Data is the largest collection of spectra that I have encountered. This library includes experimental data. You can purchase the whole collection or access it via subscription. There is no user limit.
For convenient access, you can subscribe to a web version that has a browser plugin. For increased security you can purchase and install the whole database on an internal server for faster searching and more flexible use.
### Encyclopedias & Texts

<table>
<thead>
<tr>
<th>Title</th>
<th>Publisher</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Encyclopedia of Analytical Chemistry</td>
<td>(Wiley: 2000)</td>
<td></td>
</tr>
<tr>
<td>Encyclopedia of Spectroscopy</td>
<td>(VCH: 1995)</td>
<td></td>
</tr>
</tbody>
</table>

See the handout for a listing of newer and useful encyclopedias, texts and internet sites. Some are: SLIDE
Spectroscopy on the internet

- Wiley's Spectroscopy Now
  http://www.spectroscopynow.com/Spy/basehtml/SpyH/
- Webster's Organic Chemistry
  http://ep.llnl.gov/msds/orgchem/spectroscopy.html
- Physics Encyclopedia: Spectroscopy and Radiation
  http://members.tripod.com/~IgorIvanov/physics/
- Spectroscopy Magazine
  http://www.spectroscopymag.com/spectroscopy/
- Chemistry Hypermedia Project: Spectroscopy
  http://www.chem.vt.edu/chem-ed/ac-basic.html
- ACS Division of Analytical Chemistry
  http://www.acs-analytical.duq.edu/
- Nobel Library Science Reference Room Chemistry Resources
  (Linda Shackle): http://www.asu.edu/lib/noble/chem/
Don’t feel like you always have to know all the answers. I found a few spectroscopy experts on my campus and I bet your organization has some too. Also note that many instruments are coming with built in spectra libraries. Lastly, be aware that spectral data on the internet may not be what you are expecting. For example, in the Protein Databank, Spectral Data turns out to be molecular coordinates derived from spectroscopy experiments.
We have covered a lot of ground today. In summary, spectroscopy refers to:

SLIDE
I want to acknowledge the following people for all their assistance with my talk. Thank you.