Secrets of Spectroscopy Revealed
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Robert Powers, Reporter
Jet Propulsion Laboratory Library.

Sue Cardinal (Univ. of Rochester), Reinhard Neuder (Wiley & Sons) and Larry Taylor (Bio-Rad Laboratories) talked about the basics of spectroscopy and trends in spectral databases. The talks were aimed at chemistry librarians who receive questions about spectroscopy. I found the session very helpful. I learned about changes in spectroscopy data management and retrieval, and got a nice refresher on the sources for spectral data. I was, however, left with the question about what role librarian play in this increasingly sophisticated area. Spectroscopy reference data is being integrated into instruments and data management systems, and I'm not sure what added value the library can provide.

Sue Cardinal, Chemistry Librarian for the University of Rochester, started the session, with a lot of information on "what is spectroscopy", the types of techniques that exist, and an overview of spectroscopy resources.

What is spectroscopy? It is a method used to "identify and or quantify elements, atoms, molecules, matter, molecular structure by observing absorption, emission or scattering interactions with electromagnetic radiation." Sue gave an overview of what electromagnetic radiation (EM) is, and talked about the typical interactions of EM with elements, atoms, and molecules:

- ✓ Absorption - radiation goes in, but does not come out.
- ✓ Emission - radiation is given off.
- ✓ Scattering (Raman) - the path/frequency of radiation is different them what went in.

A spectrum, is just a graphical representation of the absorption, emission or scattering of the radiation. Sue then reviewed the major spectroscopic techniques that are used by scientists.

Technique	**Definition**	**Key Parameters**	**Year**
Mass Spectrometry (MS)	Ionization and fragmentation of molecules by high energy electrons in an electric field; used to determine molecular weight	✓ Ion abundance (intensity) ✓ Mass- to- charge ratio ✓ Base peak ✓ Molecular ion (M^+)	1940's
Raman	Scattering of Infrared light due to molecular bond vibrations.	✓ Peak location ✓ Peak shape ✓ Peak strength ✓ Wave numbers ✓ Transmittance	1930's/ 1960's
Ultraviolet (UV) / Visible	Absorption of Ultraviolet and Visible light due to electrons moving to higher energy levels	✓ Molar absorptivity ✓ Extinction coefficient ✓ Maximum absorption ✓ Absorbance	1941
Infrared (IR)	Absorption of Infrared light due to molecular bond vibrations.	✓ Peak location ✓ Peak shape ✓ Peak strength ✓ Wave numbers ✓ Transmittance	1951
Nuclear Magnetic Resonance (NMR)	Absorption of radio waves in the presence of a strong magnetic	✓ Chemical shift: delta, Tau	1952

Resonance (NMR)	field used to determine molecular structure for nucleus types H, C, F, P, N.	✓ Frequency: ppm or hz ✓ Coupling constant ✓ Integrals	

Sue reviewed resources for finding articles, reference books, spectral libraries and web sites. Due to the amount of information that Sue presented on resources, I will point you to http://www.sla.org/division/dche/spectra.html for a copy of her complete presentation, and to a handout http://www.sla.org/division/dche/spechandout.html that was passed out at the session.

Sue concluded her talk by discussing the specialized software and database systems for searching, prediction, interpretation, processing, and storage of spectra. Some of the software that Sue talked about was SDBS Integrated Spectral Data Base, Sigma-Aldrich, ACD Lab, NIST Web Book, BioRad's - KnowitAll/HaveitAll, and Wiley Chemical Concepts - SpecInfo.

Reinhard Neuder of Wiley & Sons talked about the "Secrets of Structure Elucidation and Spectroscopic Databases". Laboratory automation and combinatorial chemistry have increased the volume of spectra data that needs to be analyzed. Spectroscopic databases such as SpecInfo help to automate the analysis of this data. SpecInfo allows the user to search by inputting a spectrum, and the database will search for a compound, or you can predict the spectrum for a given compound. Reinhard conducted a tour of the SpecInfo product, and highlighted its features via a number of case studies. Finally, Reinhard demonstrated the hypertext links that Wiley has implemented in some of its journals, between electronic journal articles and SpecInfo.

Larry Taylor of Bio-Rad Laboratories rounded off the session with a presentation on "Spectral Database Libraries: Creation, Management and Access". Larry made the point that spectral libraries use to be multi-volume reference books in the library. Today, the libraries are sophisticated databases made of digitized spectra, instrument parameters, structures, and physical and chemical properties. Many users of these databases supplement publicly available spectral data with proprietary data. Therefore, many of the database products allow the user to build and manage their own in-house database. Much of Larry's talk was technical, and focused on the creation and management of spectral databases, costs, when to build vs. off the shelf, and database architecture. Much of this information was interesting, but not really applicable to librarians. Or is it? As I mentioned above, I did wonder what the role of the information professional (librarian) is as the information technology improves.