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"Making Connections Between Spectroscopy and General Chemistry. A Series of Practical Exercises"

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Abstract

Reasons for including spectroscopy experiments and activities in General Chemistry are discussed. Suggestions are given on how to incorporate spectroscopy activities in the general chemistry syllabus. Spectroscopy experiments and activities are described. Sample spectroscopy based experiments are provided. Sources of simulation software and references are given for some spectroscopy experiments specifically developed for general chemistry.

Why include spectroscopy in general chemistry?

How can spectroscopy be included in general chemistry?

Some practical spectroscopy activities for general chemistry.

Some spectroscopy resources

Why include spectroscopy in general chemistry?

I am a physical chemist and did my thesis research using electron spin resonance. I think that spectroscopy is an exquisite probe, and that its application to our everyday lives is widespread.

I teach at Bellevue Community College, a large urban community college. Because the chemistry department is small, I have taught every course in our curriculum, from chemistry for non-science majors to the year-long sophomore organic sequence, although for many years I have been mostly teaching organic chemistry and General Chemistry. Knowledge of spectroscopy is essential when working with organic chemistry and when I began teaching organic chemistry, I was surprised that most students had not been introduced to spectroscopy at all in their General Chemistry course. A few students had experience with colorimetry and atomic emission spectra, but absorption was new to almost everyone. Most had never studied infrared, UV-visible or NMR spectroscopy and had no experience with absorption spectra at all. The General Chemistry courses omitted discussion of these key topics. This is a reflection of the content of many General Chemistry texts. Popular General Chemistry texts typically discuss spectroscopy only associated with atomic emission spectra and crystal field theory applied to complex ions. This usually amounts to 10-15 pages in books that have swollen to 1000 pages. I believe there is a mismatch here. There is an imbalance between traditional topics and modern ones.

General Chemistry has the largest number of students of any of the classes in the chemistry curriculum. It serves to introduce thousands of students to the field of chemistry. All of the future engineers, dentists, doctors pharmacists take General Chemistry. Many of these professions require students to continue on with organic chemistry. Some do not. This means that a large number of students will only see chemistry through the view of a General Chemistry window. Their vision of chemistry will be forever shaped by their experience in General Chemistry. To me this means General Chemistry students need more than the traditional emphasis on basic atomic structure, stoichiometry, gas laws, and equilibrium calculations. The "spiral" approach to teaching chemistry is used for most other topics but not for spectroscopy.

It may sound strange to describe a college with 17,000 students as small. The fact is that although we have a student

population of 17,000, only a hand-full of the 17,000 students take any chemistry at all. Even fewer take General Chemistry. Our General Chemistry enrollment is a mere 176 students in fall quarter followed by another cohort of 120 in winter quarter with another 24 in a summer session. The total is about 300 students each year. The number of students who continue on and start organic course is even smaller. We have only 48 students in our sophomore organic chemistry. This is about 16% of the students who started General Chemistry.

Is this an unusual situation? I know that a similar pattern exists at the University of Washington. In 1998-99 about 2100 students started General Chemistry. This number dwindled to about 850 who started sophomore organic chemistry. This means only about 40% of the students who started General Chemistry go on to start sophomore organic chemistry. The percentages are different for the two colleges partly because some students from the community college transfer to four year schools for their sophomore year.

To me this indicates that General Chemistry is frequently the first and, in many cases the last, set of classes where students will be engaged in work that uses the principles of modern chemistry. This means we must introduce General Chemistry students to the concepts of spectroscopy or they may never see them. Infrared, ultraviolet-visible, NMR spectroscopy are integral parts of modern chemistry and should be incorporated into the General Chemistry syllabus so students get an accurate picture of some of the tools that are used by chemists. It seems that spectroscopy that has been around for more than 40 years or almost three generations should have some place in the basic General Chemistry course.

Most General Chemistry texts talk about spectroscopy only when emission spectra of atoms and energy levels are discussed. General Chemistry texts often only mention spectra when discussing atomic emission spectra. The present emphasis on stoichiometry, titrations, redox potentials, acids and bases deals with a limited set of information. It gives a distorted image of what is done in chemistry.

Spectroscopy provides information that is at the base of some very abstract ideas in General Chemistry. In many texts students are offered little experimental evidence for many topics about bonding. A rudimentary experience with spectroscopy can help students visualize current models of molecular motions, differences in bonds, energy levels in molecules, resonance, hydrogen bonding, color, etc.

There are a large number of experiments that have been written for use in General Chemistry. These are excellent experiments, but often they require instrumentation that is unavailable to financially-challenged departments. Even well-funded departments may have logistical problems when huge numbers of students are enrolled in labs. This creates a situation where simulation software can provide students experience without the need for additional lab space or large numbers of instruments. A combination of simulation software and hands-on instrument use would be ideal. If the hardware is not available at least students should be able to gain experience using simulations and spectra libraries.

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Reasons for including spectroscopy in General Chemistry

I believe that there are at least three significant reasons for including spectroscopy related activities in General Chemistry.

1. About sixty percent of General Chemistry students do not continue with any more chemistry. This means that they will have almost zero experience with spectroscopy if it is omitted from the General Chemistry syllabus. In this situation successful General Chemistry students will not know any more about absorption spectra, infrared spectra, NMR and ultraviolet spectra than students who never took a chemistry course.

2. Students who do go on to organic often have great difficulty. One of the major tools of organic chemistry is spectroscopy. If General Chemistry includes a brief exposure to the concepts of IR, UV-visible and NMR, students may have a better chance of understanding the principles they encounter in organic chemistry.

3. Techniques of modern medicine are increasingly dependent on what we chemists call "spectroscopy" such as CAT scans, MRI's, etc.

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How can spectroscopy be included in General Chemistry?

Right now you may be saying, "General Chemistry is already overloaded with content. Where will spectroscopy fit? What will have to be dropped from the course? " I believe nothing need be dropped. A shift in emphasis may be needed. The amount of time spent on traditional topics could be altered.

I believe that spectroscopy fits well when discussing bonding and molecular shapes. When I teach General Chemistry, I always introduce IR spectroscopy during the discussion of bonding. We have a small chemistry department with a limited budget. I know that we cannot afford to purchase and maintain both an FTIR and FTNMR spectrometer. Therefore, I have adopted the strategy of introducing students to these topics using small libraries of spectra and simulations. Specifically we have used IR Tutor(1), IR Simulator (2), Beaker(3), and the Journal of Chemical Education proton nuclear magnetic resonance simulator program. Relatively inexpensive software and spectral libraries can be used to provide spectra.

Spectroscopy also can be included as part of a project during the second semester or third quarter of the General Chemistry series. I have used a project that is centered on an organic synthesis. Students examine IR and NMR spectra for reactants and products in a one step synthesis of benzil from benzoin.

Students do a microscale synthesis and determine their melting point and percent yield. They do an analysis of NMR and IR spectra for reactant and product. I provide IR spectra for the reactants and products. Students use an NMR spectrum simulator program to generate the NMR spectra. They are asked to assign chemical shifts to protons in the structures of reactants and products. We have an FTIR now and students can record their own IR spectra. This is a good experience, but not an essential one. Students have three weeks to complete the project and submit their project report.

NMR simulated spectra are a great tool for demonstrating how electronegativity influences shielding and electron density in molecules for General Chemistry. I introduce the class to PMR and chemical shifts. Students then use a NMR simulator program to generate spectra for a hydrocarbon and a series of halogenated compounds. The effect of the halogens on the chemical shift can be examined. Students can see the change in shielding as the number of halogens change. They "see" the effect and are very impressed. The students seem to feel they are dealing with modern aspects of chemistry and enjoy the idea of manipulating molecules while working with the simulator program.

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Examples of spectroscopy related activities for General Chemistry

1. A Basic flame test and emission spectra exercise for Introductory Chemistry
2. IR identification of an unknown.
3. UV electronic spectra
4. Chemical shifts, electron density and electronegativity
   to be linked later

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Some spectroscopy resources

Infrared Pages on the Net

Please send comments and suggestions for additions/modifications to Lodder@pop.uky.edu
Click below to go to a specific section of the list: Laboratories and Departments

http://kerouac.pharm.uky.edu/asrg/cnirs/ir_spec.htm#labs

Commercial Instrument Manufacturers and Other Companies

http://kerouac.pharm.uky.edu/asrg/cnirs/ir_spec.htm#comps

Personal Home Pages of IR Spectroscopists

http://kerouac.pharm.uky.edu/asrg/cnirs/ir_spec.htm#people

Courses and Tutorials

http://kerouac.pharm.uky.edu/asrg/cnirs/ir_spec.htm#tuts

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Encyclopedia of Analytical Instrumentation

Software and other Resources / Data Acquisition and Electronics / Data Handling / Diffraction / Electrochemistry / Gravimetry /Imaging / Mass Spectrometry / Materials & Surface Analysis / Optics / Sensors / Separations / Spectroscopy /Standards / Thermal Methods / Titration

http://www.scimedia.com/chem-ed/analytic/ac-meths.htm#spectroscopy

Web sources for information regarding NMR simulation software

A Compilation of Educational NMR Software

Peter Lundberg

Magnetic Resonance unit, Dept of Diagnostic Radiology, Linkoping University Hospital, S-581 85 Linkoping, Sweden.

(Previous address: Dept of Physical Chemistry, University of Umea, S-901 87 Umea, Sweden)

Preferred email address: PeterL@mr.us.lio.se (alternative address: Peter.Lundberg@chem.umu.se)

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Proton NMR Basics

A multimedia presentation of the basics of NMR spectroscopy. On CD-ROM with

QuickTime movies and animation.

Four sections: Introduction (What is the use of NMR?); The instrument room (demo of a spectrometer); The classroom (analyzing simple spectra); Laboratory (spectra of complex molecules) CD-ROM for Macintosh and PCs.

Available ($60) from JCESOFT at http:// jchemed.chem.wisc.edu/JCESoft

By CS Judd, JD Morrisett, MV Chari, JL Browning.

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NMR concepts with MathCad

MathCad documents demonstrating NMR concepts. Introduction to NMR, quadrature detection, phase cycling, apodization.

For MathCad (PCs). Viewer available.

Free programs from http://science.widener.edu/svb/nmr/nmr.html

By Scott Van Bramer (svanbram@science.widener.edu).

Fourier transform with MathCad

MathCad documents showing how the Fourier transform is used in NMR spectroscopy. Introduction, two signals, real and imaginary spectra, and decaying signal.

For MathCad (PCs).

Free programs from http://science.widener.edu/svb/nmr/nmr.html

By Scott Van Bramer (svanbram@science.widener.edu).

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Proton NMR Simulator

A program for simulating proton NMR spectra on a Mac. Draw the structure on screen and the spectrum will be displayed at

60-360 MHz. Clicking on a hydrogen in the molecular structure indicates the multiplet generated by that hydrogen, and clicking on any peak in the spectrum highlights the corresponding hydrogen in the molecular structure drawing. Very easy to use.

For Macintosh.

Available ($50) from JCE Software (Kersey Black, Proton NMR Spectrum Simulator, JCE Software, 1990 , Volume IIc, No. 1).

Email: JCESOFT@MACC.WISC.EDU By Kersey Black.

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Raccoon

Program for simulation of spectra at different field strengths ("Really Awesome Computer Calculation Of Observed Nmr spectra"). Up to 7 spins, plus additional singlets, and optional noise, integration, printing on most printers, etc (in the updated version). Easy to use.

For PCs (DOS)

Available from project Seraphim (the old 1984 version), at $20 (disk PC4101) with a few more programs. Email: JCESOFT@MACC.WISC.EDU. Free program Raccoon II (the new Version 2.1, 1993) from Hans Reich (email: REICH@chem.wisc.edu).

By Paul Schatz, and Hans Reich.

Calleo NMR

A spectrum simulation program (version 1.0 for Mac) for all naturally occuring isotopes for the first 103 elements. You can select the isotopic abundance etc. 8 spins, dipolar coupling, etc.

For Macintosh.

Distributed by Calleo Scientific Software Publisher, 3951 Braidwood Dr, Fort Collins, Colorado 80524, Ph (970) 482-9745. Price $275-375 . (www: http://members.aol.com/calleo, Email: calleo@aol.com)

By AK Rappe from the Colorado State University, and CJ Casewit of Calleo.

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A partial list spectroscopy experiments for General Chemistry

Abney,-James-R.; Scalettar,-Bethe-A., J. Chem. Educ. 1998, v75 n6 p757-60.

Describes absorption spectroscopy experiments that allow students to explore the mechanisms by which sunscreens and sunglasses provide protection from ultraviolet radiation. Exposes students to absorption phenomena in an engaging way.

Ackermann,-Martin-N., J-Chem-Educ. 1970, 47, 1, 69-70.

Describes a General Chemistry experiment which uses infrared spectroscopy to analyze inorganic ions and thereby serves to introduce an important instrumental method of analysis. Presents a table of eight anions and the ammonium ion with the frequencies of their normal modes, as well as the spectra of three sulfate salts.

Bosma,-Wayne-B., J. Chem. Educ. 1998, v75 n2 p214-15.

Describes a set of experiments using a UV-VIS spectrometer to identify food colorings and to measure the pH of soft drinks. The first laboratory component uses locations and shapes of visible absorption peaks as a means of identifying dyes while the second portion uses the spectrometer for determining pH.

Shalhoub,-George-M., J. Chem. Educ. 1980, v57 n7 p525-26.

Describes an experiment for General Chemistry that illustrates the use of spectroscopy in the synthesis, characterization, and nitration of tris(acetylacetonato)cobalt (III).

Reedijk,-J.; and-others, Education-in-Chemistry, 1975; 12, 4, 113-114.

Describes an experiment, for the General Chemistry laboratory, intended to introduce the student to infrared spectroscopy. After being introduced to the theory of molecular vibrations on an elementary level, each student receives a list of 5-7 nickel (II) ammines to be prepared, analyzed and characterized by infrared spectoscopy.

Potts,-Richard-A. J. Chem. Educ. 1974, 51, 8, 539-540.

Describes a series of experiments designed for General Chemistry in which the students prepare metal complexes which are then used as samples for spectral study.

Williams,-Gregory-M.; and-others. J. Chem. Educ. 1989, v66 n12 p1043-45.

Described is an experiment involving the synthesis and spectral studies of cobalt complexes that not only give General Chemistry students an introduction to inorganic synthesis but allows them to conduct a systematic study on the effect of different ligands on absorption spectra. Background information, procedures, and experimental results are discussed.

Magyar,-Elaine; Magyar,-James-G. J. Chem. Educ. 1989, v66 n3 p245-46.

Investigates the four week chemistry program in a summer program in science and mathematics. Identifies weekly topics for the program: (1) color and visible spectroscopy; (2) UV spectroscopy, fluorescence, and chemiluminescence; (3) IR and NMR spectroscopy; and (4) lists 12 individual projects.

Steinert,-Roger; Hudson,-Bruce. J. Chem. Educ. 1973, 50, 129-130.

This transition, observed with an inexpensive ultraviolet photometer, is a potentially useful experiment for an advanced freshman class because it introduces several concepts of general

physical interest.

Daines,-Terri-L.; Morse,-Karen-W. J. Chem. Educ. 1976, 53, 2, 126-127.

Describes an experiment which quantitatively determines glucose by a spectrophotometric measurement of the colored complex formed between glucose and an amine.

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