BRINGING VIBRATIONAL SPECTROSCOPY INTO THE GEOLOGY CLASSROOM

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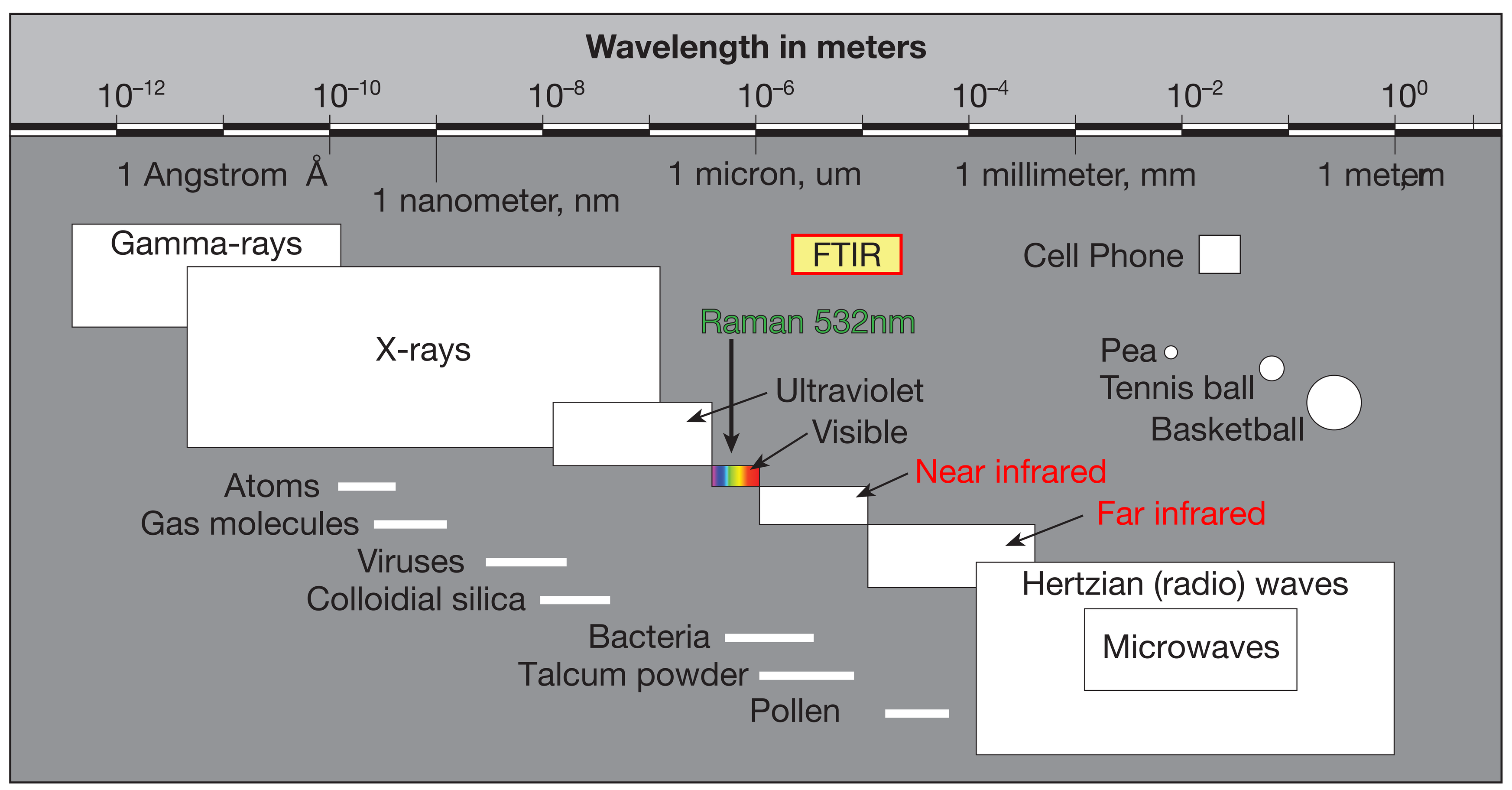
Abstract

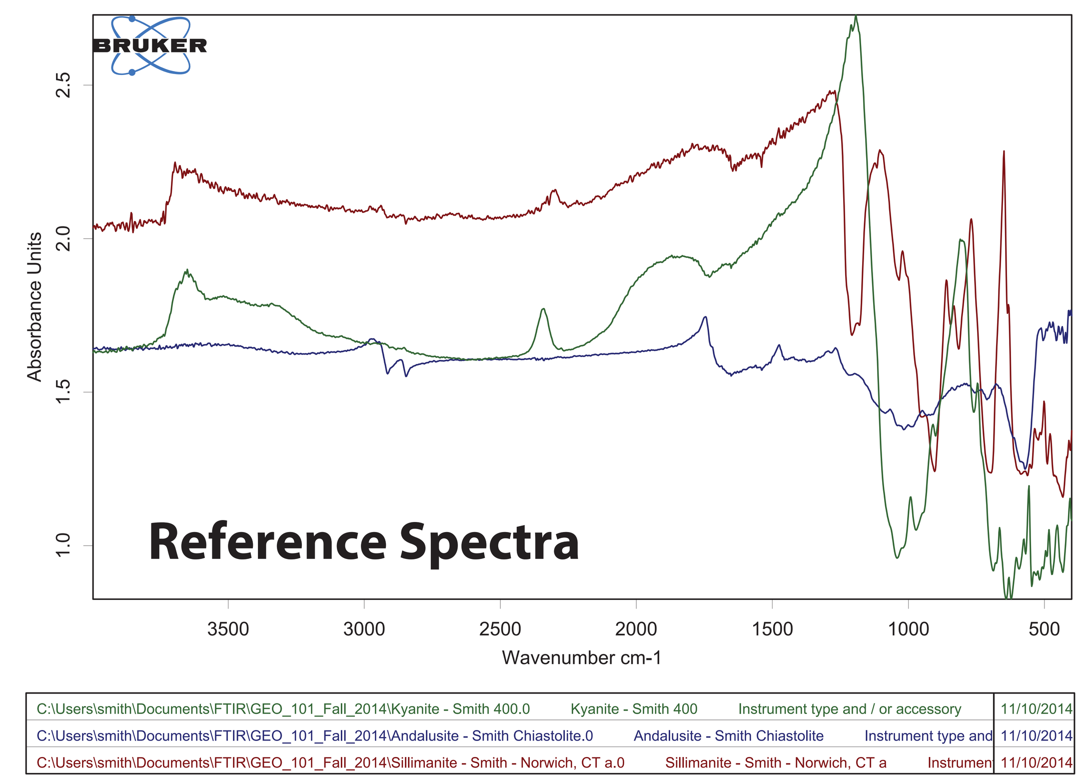
Fourier transform infrared (FTIR) spectroscopy and Raman spectroscopy are increasingly used by geoscientists and others in their research. Recent advances in the development of commercially available Raman and FTIR spectrometers now make this technology accessible to students and faculty in the geosciences for whom spectroscopy has not traditionally been a focus. These spectrometers are powerful tools that significantly expand our capability to identify and characterize geological materials and provide excellent opportunities to build analytical competence through their careful use in geoscience curricula. We are exploring the use of vibrational spectrometers in our courses and report here on our initial experiences using an FTIR spectrometer in introductory geoscience classes. In particular, we are using the Bruker Alpha™ benchtop FTIR with several of their QuickSnap™ sampling modules for hand samples (reflection module), powders (ATR module), and gems or chips (diffuse reflection module). Data collection is easy for students with little training. Mineral identification can be confirmed by students through comparison with standard spectra, either manually or using the Bruker OPAL™ software. For best results, we have created standards libraries with a limited number of minerals both with RRUFF (www.rruff.info) files and with data collected on the samples in use. Students report that they like the identification clarity that the spectrometers typically provide and feel frustration when the spectra are not sufficiently unique. We use the activities involving the spectrometers to introduce additional concepts about crystal structures and the vibrational energies of bonds. Our plan is to build on these concepts with more in-depth spectroscopic work in intermediate and advanced courses. Come to our poster to use the FTIR spectrometer, which is portable enough to bring to NE GSA.

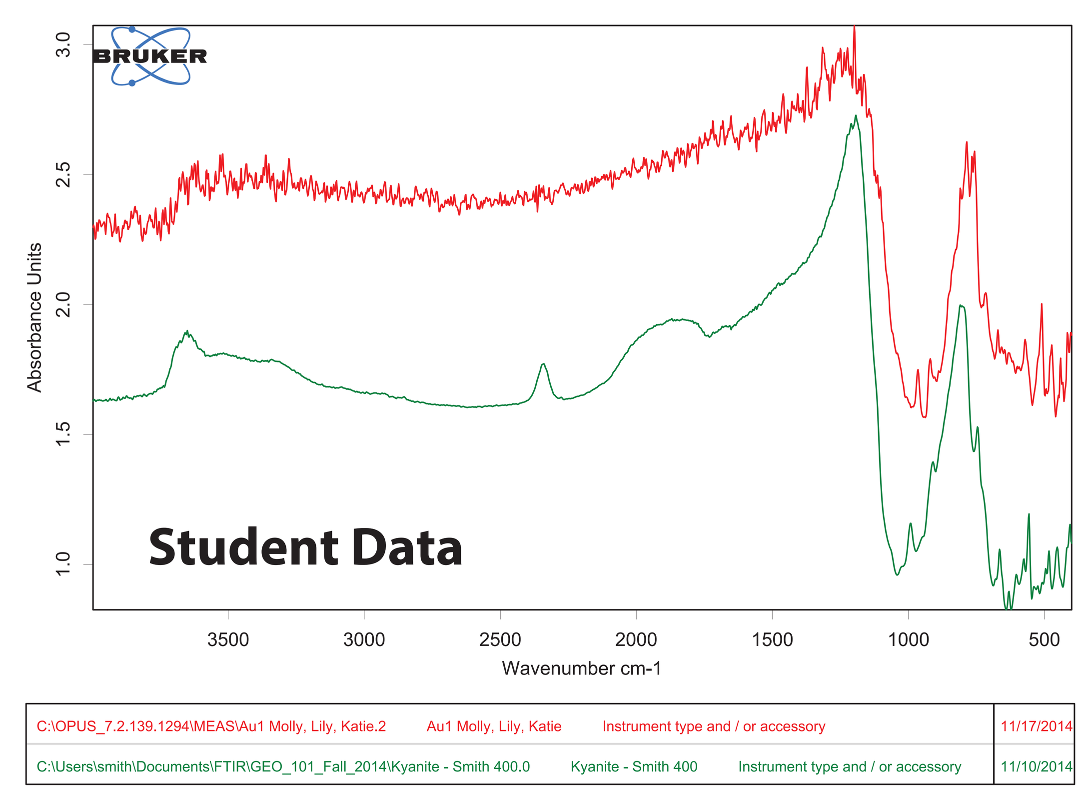


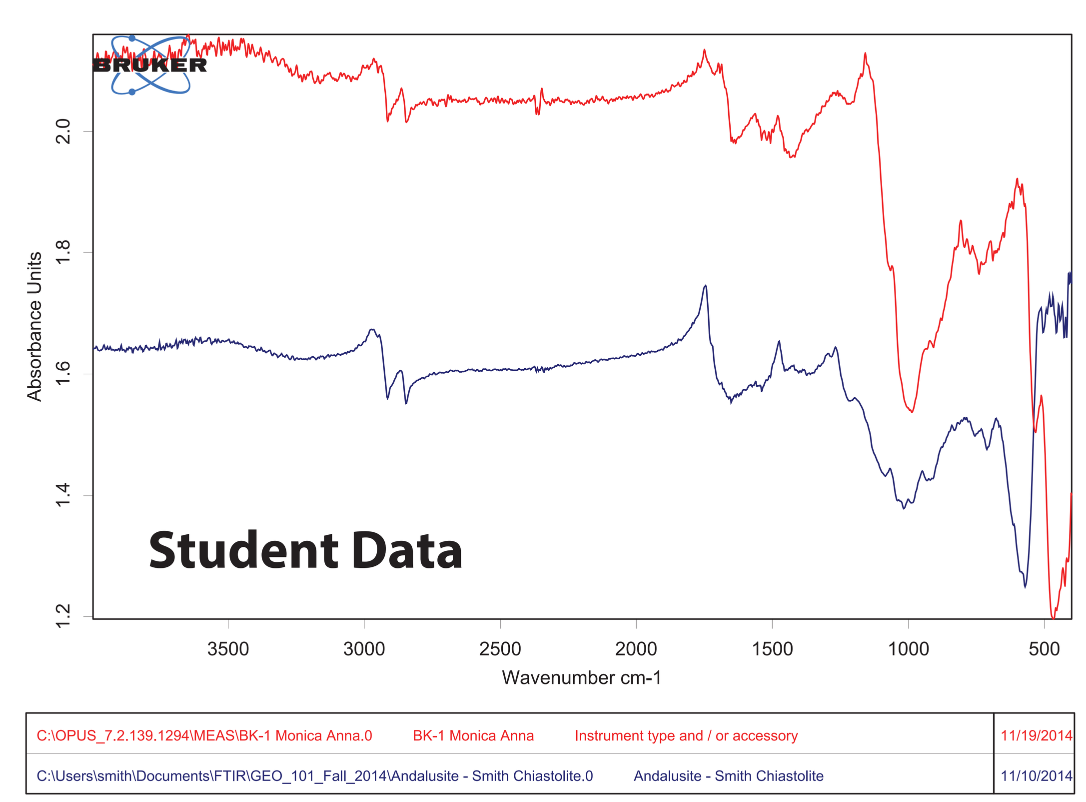
Remember these Points for the Poster Quiz

- Because more and more geologic researchers are using spectroscopic methods, it is important that our students are exposed to spectroscopy early in their careers to prepare them to understand scientific data.
- FTIR spectrometers are comparatively easy to use for identification of minerals, and we have used them successfully in introductory geology classes.
- FTIR spectrometers are "inexpensive" (~$25,000), compact, and safe.
- FTIR spectroscopy provides an analytical confirmation of mineral identification that compares favorably with powder x-ray diffraction.
- Issues of sample preparation and of mixed spectra due to multiple minerals in the sample are similar to those that affect powder x-ray diffraction.
- Bench-top Raman spectrometers can be used in a manner similar to bench-top FTIR spectrometers with similarly good results.
- Safety protocols required to use the better bench-top Raman spectrometers with Class IIIB lasers (>5mW power) add a level of complexity that must be considered when choosing among the two spectrometer types.
- Because both FTIR and Raman spectrometers give good data for organic solids and liquids as well as for inorganic crystals, and because both spectrometers are relatively portable, sharing instruments with chemistry colleagues is realistic.

Class Example: Identifying Aluminosilicate Polymorphs



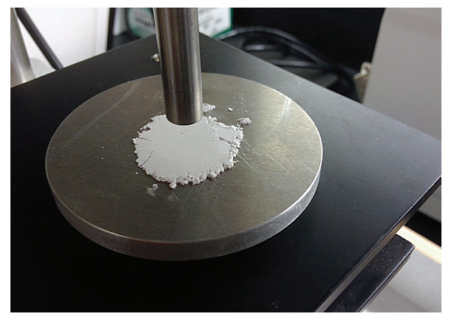




Spectroscopic Activity Examples

Name That Mineral
asks the introductory students to identify samples from a group of common rock-forming minerals using Raman and FTIR.

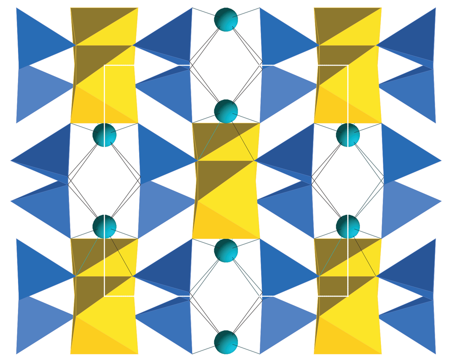
What's That White Powder?
asks students to become forensic scientists and identify the mineralogy of common white substances, including baby powder, blackboard chalk, rock-climbing chalk, and wall-board.



Gemstones: Let the Buyer Beware
lets student use both Raman and FTIR to compare the spectra of naturally-occurring vs. treated gemstones, becoming familiar with the effects and associated spectral signatures of the various treatments.

Mineral Synthesis and Breakdown
helps students develop the concept that minerals can be both the products and reactants for chemical reactions, and that these are chemically linked. Students will learn to design, execute, and evaluate synthesis and/or decomposition experiments using Raman and FTIR.

Twist and Turn: The Geometry of Molecules in Minerals
is a series of experiments on minerals from which students will collect Raman spectra in various crystallographic orientations. Optical characteristics of several minerals in the same array of orientations will be examined, providing the opportunity for students to synthesize concepts about the interaction of visible light and laser light with lattices, the geometry of molecular groups within lattices, and the information derivable from multiple analyticaltech niques.



Pottery and Glazes: Before and After Firing
will examine the minerals used in pottery and in glazes and the changes they undergo during the firing process. This experience can then be applied to the study of pottery from various sources, as used by art historians and archeologists.

Questions Geology Students Should be able to Answer After these Activites

- What is the ectromagnetic spectrum?
- What is infrared radiation?
- Is infrared radiation dangerous to humans?
- How is energy related to wavelength for electromagnetic waves?
- What are the axes of an FTIR spectrum?
- How are wavenumbers related to wavelengths?
- What causes the peaks and valleys of an FTIR spectrum?
- Can mineral samples can give FTIR spectra?
- Will materials that are not minerals give FTIR spectra?
- How are the samples prepared? Does it matter?
- Why is a background spectrum collected? How is it used?
- Why are the FTIR spectra from different minerals unique?
- Why are the FTIR spectra from different samples of the same mineral very similar?
- Why are the FTIR spectra from different samples of the same mineral not identical?
- When should one use FTIR as an aid in mineral identification?
- How might the bonds causing infrared adsorption be identified?