2014

2014 Research at Andrews

Andrews University

Laser Blasting

Spectroscopy as an Educational Tool for Chemistry and Biochemistry Students

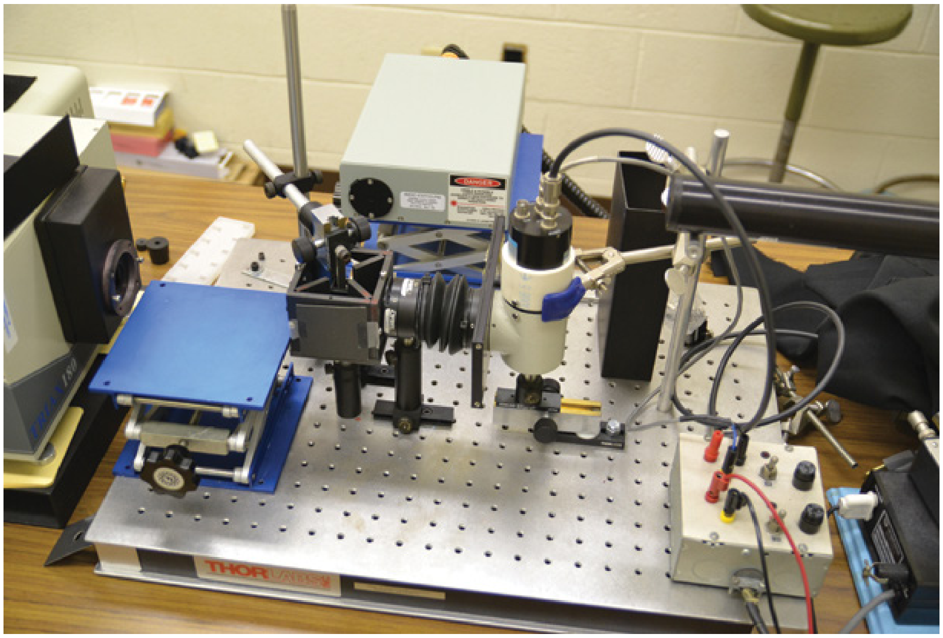
Everyone loves the moments on television when crime scene investigators test a substance, point to their computers and say, "a-ha, it was arsenic." But how did they actually know? What happened between the moment when they tested the substance and the answer flashed on their computer screen? David Randall and Ryan Hayes, professors of chemistry at Andrews University have the answer: spectroscopy!

Spectroscopy studies the interaction of light (electromagnetic radiation) with matter. The wavelengths of the light that are transmitted, absorbed or reflected are then analyzed in order to learn about the substance.

"Basically, spectroscopy is a standard method for chemists and physicists to figure out the identity of materials," explains Randall. "From an analytical chemist's perspective, there are two domains of spectroscopy: one analyzes molecules and the other analyzes atoms." Randall and Hayes became involved in spectroscopy as undergraduate students at Andrews University in Dwain Ford's organic chemistry course. Randall continued using spectroscopy during his graduate work at the University of California, Davis as did Hayes, who completed his doctorate at Northwestern University.

Hayes and Randall are fascinated with finding out the makeup of materials using spectroscopic techniques. Hayes is currently researching the structure of arginine-based heterocyclic amines which are potential carcinogens created in very low quantities when plant proteins are overcooked or charred. Using UV-VIS absorbance, fluorescence, nuclear magnetic resonance (NMR) spectroscopies, Hayes and student researchers are determining the molecular structure of these potential carcinogens which have not been previously discovered and published. Hayes is also collaborating with fellow chemistry professor Desmond Murray and student researchers on the use of stilbenes as a fluorescent detector of metal ions, namely copper(II) ions. This research uses the same three spectroscopic methods listed above. Hayes has mentored students who have participated in his research projects as undergraduate research scholars and several honors theses have been produced as a result.

The spectrometer ready for action **PHOTO:** *David Randall*



Randall is developing a nitric oxide (NO) sensor with student researchers in order to determine the amount of NO in a specific solvent. He is also involved in an interdisciplinary project with biology professor Peter Lyons and physics professor Brendan Cross, who are analyzing the protein folding mechanisms of carboxypeptidase O using Fourier transform infrared (FTIR) spectroscopy. Randall's previous research projects include a spectroscopic study of enzymes that contain metal-ions using the spectroscopic methods of electron paramagnetic resonance, resonance Raman, and magnetic circular dichroism.

This enthusiasm for problem solving and analysis has spread to their teaching methods, particularly when it comes to spectroscopy. When Randall and Hayes began working at Andrews, they started utilizing a lab-built Laser Induced Breakdown Spectroscopy (LIBS) instrument that was assembled by one of Dwain Ford's colleagues, Peter Wong (now professor emeritus of chemistry). Wong had purchased a neodymium doped yttrium aluminum garnet (Nd:YAG) laser with funds he secured from a Dreyfus Research Award (matched by Andrews University). Rather than buying a LIBS spectrometer as a dedicated unit, Wong assembled one from individual parts.

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Purchasing a complete unit could cost close to $90,000. On the other hand, the cost of purchasing and assembling the readily

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available parts from scratch costs under $30,000, a savings of $60,000. Additionally, the laser, which is the bulk of the expense, can be repurposed for other experiments and research.

According to Randall, Wong set up a model for using spectroscopy in general chemistry and upper division classes that Randall and Hayes now teach. They have continued the tradition of using the spectrometer in the classroom as a teaching tool. “Our contribution was documenting the use of spectroscopy in the classroom and putting it in a paper. Dr. Wong implemented the instrument and the labs to go with it,” says Randall.

In 2013, Hayes and Randall published an article with Peter Wong entitled “A simple LIBS spectrometer for use at multiple levels in the undergraduate chemistry curriculum” in the *Journal of Chemical Education* 2013, 90(4), 456–462. The main purpose of the article was to document how to put together a simple

David Randall

Ryan Hayes

LIBS spectrometer that could be used in undergraduate classes. “It’s a template for how to set up the spectrometer yourself,” explains Randall. The article describes what parts they used to construct the spectrometer, how to conduct experiments, and how to use the module in the classroom. At a national American Chemical Society meeting, where Randall was presenting a poster on this, a faculty member from Centre College in Kentucky said that he was able to use the article to give a project to one of his students.

In addition to the cost savings and flexibility mentioned above, a modular spectrometer like the one Wong assembled teaches students how all the parts of a spectrometer work together and also gives students practice using standard research equipment. “One of the things that is really excellent about Dr. Wong’s component-based instrument style is that when students leave Andrews, they actually understand how the instrument works, they aren’t just pushing buttons and operating a black box,” he says. Students use the instrument to learn the step-by-step process of how scientists identify the elements in a sample and how the major components of the instrument work together. By using a spectrometer in the chemistry lab, “it helps to demystify how scientists figure out what is inside of something,” says Hayes.

The LIBS technique that Hayes and Randall use is a type of atomic emission spectroscopy. The nanosecond pulsed laser they use is so powerful that it produces plasma at around 10,000K (the surface of the sun is around 6,000K). This high temperature blasts and atomizes material from samples, such as a piece of Pepto-Bismol or a paint chip, which are mounted in the sample holder. The sample holder sits at the focal point of a 5.0 cm focal length lens that focuses the laser beam onto the sample. This excites the electrons in the sample, which then emit light as they return to their ground state electron orbitals. A detector integrated with a spectrometer is attached to a computer and records the spectrum of light emitted from the sample. Control software collects spectra, allowing students to observe the wavelengths of the peaks from the sample and compare them to peak wavelengths of known standards, such as elemental bismuth or lead.

“When you blast the sample with this high-powered laser, it’s so powerful that if you put in a blank card it makes a snapping sound that comes from the expansion of rapidly heated air,” says Randall. To help protect students and faculty, Hayes covers the equipment with a black cloth to make sure no light gets in or out during the experiment.

Once the equipment is set up, the whole experiment takes no more than five minutes. “Because there is minimal sample preparation, it’s a very fast way to determine what is in the sample. A limitation of our instrument is that it is not quantitative. It doesn’t tell us how much of a given element is present; only that it is present,” says Randall.

To make the class experiments interesting, Randall and Hayes have created scenarios where students play the role of forensic scientists. According to Hayes, this helps them understand that what they see in popular forensic television shows is not entirely accurate. Instead of the answer popping up on the screen, there is actually a process that scientists have to go through in order to get the answer.