Interdisciplinary Science Technology- Raman Spectroscopy to Meet the State and National Teaching Standards

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ABSTRACT

Students need to be engaged into the lab with real-world instrumentation such as Raman spectroscopy which is highly needed into today's technological world. This study has engaged undergraduate students into problem solving the organic structure of various compounds /functional groups by utilizing i Raman spectroscopy instrumentation. The students understanding of abstract bonding concepts has been utilized by the FBI to solve and analyze unknowns /forensic chemistry compounds of interest. These experiences with the hands-on instrumentation have shown enhanced test scores in organic chemistry as well due to real-world bonding problems being resolved to analyze the unknown organic compounds by Raman spectroscopy.

Keywords: Organic compounds, octet rule, inquiry-based learning, Raman spectroscopy, technology.

1. INTRODUCTION

One of the greatest challenges of teaching chemistry has been to grasp the students' interest in a lab experiment. Many lab experiments or research projects are not engaging the students to learn how the technique or instrumentation would be utilized in a real-world setting. As a science educator the overriding goal is to engage pre-service and in-service teachers with the needed technology to solve problems in the chemistry lab setting. The most appealing experiments for students have been forensic science where students are engaged in the process of solving a crime and identifying the unknown substance. In the nature of forensic examination: transfer, identification, classification, association and reconstruction shape the field of study which depend on analytical chemistry techniques/technology. The analytical technique that was utilized in this inquiry-based lab was Raman Spectroscopy instrument to engage our pre-service and in-service teachers with understanding organic chemistry functional groups while identification of unknown samples.

Wilbur Wright stated, "It is possible to fly. But not without knowledge and skill." Our pre-service and in-service teachers were required to develop interdisciplinary knowledge by integrating organic chemistry content with the Raman spectroscopy instrument to solve the bonding /functional group identification. The **Ohio Learning Standards and Model Curriculum**, K-12, May 2019, and **Next Generation Science Standards (NGSS)** all advocate cooperative, inquiry-based science classroom with technology. The novel Raman spectroscopy technology allows our students to determine what organic functional group or groups are present in the sample and determine the actual compound integrated with a library index program. The advantage of Raman spectroscopy lab allows our students to understand the real world setting of potential value in the qualitative and quantitative analysis of trace amounts of drugs /illicit substances on different matrices such as cloth, currency notes, and fiber without the need of extensive sample preparation in a non-destructive manner.

2. INSTRUMENTATION/OVERVIEW

Raman spectroscopy involves directing monochromatic light source such as laser onto the sample and detecting the scattered light. Majority of the light scattered elastically called Rayleigh scatter, and the small fraction of light scattered inelastically is Raman scatter. Thus, Raman is based on the inelastic scattering of radiation that interacts with the substance/sample. The graph/spectral data obtained by the Raman scattering is due to the vibrational modes of the molecule. Thus, the Raman scattering (inelastic scattering) provides information about the molecular vibrational structure and can be used to identify the functional groups. The Raman instrument allows for rapid, nondestructive to sample and can be used for analysis of many classes of hazardous and potentially explosive compounds. Raman spectroscopy is sensitive to slight differences in chemical structure/functional groups which has been used to determine medicinal samples (tablet or gel cap). The Raman spectra illustrates a number of peaks where the intensity and wavelength position of the Raman scattered light. Every peak designates to a specific molecular bond vibration such as C-C, C=C, C-H and groups of bonds such as C_6H_6 ring mode, and polymer chain vibrations. The general Raman spectrum provides a unique chemical fingerprint that can be used to identify an unknown chemical sample and a comprehensive Raman spectral library search assists in providing the chemical identification, The Raman spectrum is unique to a material/sample thus it is an excellent technique for identifying unknown compounds.

3. EXPERIMENTAL

In preparation for the Raman Spectroscopy unknown sample analysis, students were required to read the PeakSeeker Raman Spectroscopy operation manual.

Safety when working the laser was utmost importance:

-Caution – use the controls or adjustments or performance of procedures other than the directions specified in the manual may result in hazardous radiation exposure.

-Do not point the laser or allow the light to be directed or reflected toward people or reflective objects.

-Always wear appropriate protective eyewear.

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-Do not modify or remove protective covers.

-Never operate laser if unit is defective or if safety covers, locks, and labels are damaged or missing.

The PeakSeeker Raman has compact dimension as shown in Figure 1., the laser probe is available in 785 nm.

<u>Figure 1.</u> Raman Spectroscopy Instrument

4. RESULTS/DISCUSSION

Raman spectroscopy is complementary to infrared (IR) spectroscopy, which depends on the change in dipole moment during the vibration, and thus offers many advantages. The following are among the analytical advantages of Raman spectroscopy:

-Little or no sample preparation is required.

-Raman is relatively unaffected by strong IR absorbers like water, CO_2, and glass (silica).

-No special accessories are needed for aqueous solutions because water is a weak scatterer.

-Fiber optics of varying lengths can be used to transmit the excitation laser light and collect the back-scattered light for remote analyses.

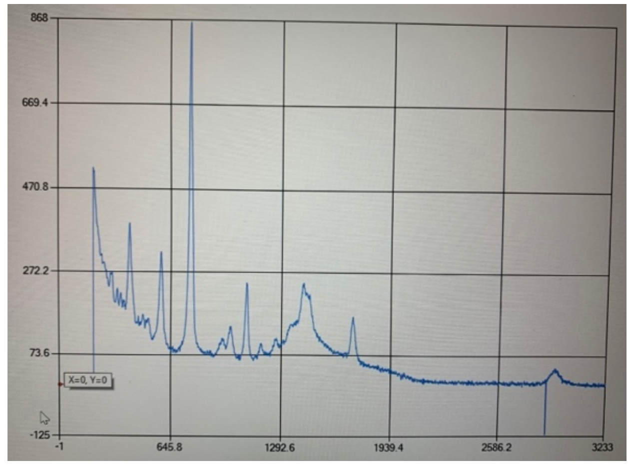
-The short wavelength excitation source can penetrate transparent and translucent container materials, and thus Raman measurements can be acquired through glass vials, envelopes, plastic bags, and several other (but not all) packaging materials.

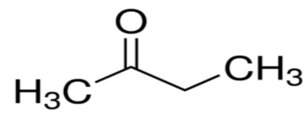
-Properties of the laser sources make it relatively easy to probe micro-samples, surfaces, powders, films, solutions, gases, and various other sample types.

- Raman systems are flexible to miniaturization for field applications.

Raman spectroscopy is a well-established analytical technique, and new portable systems are utilizing the many advantages for field applications.

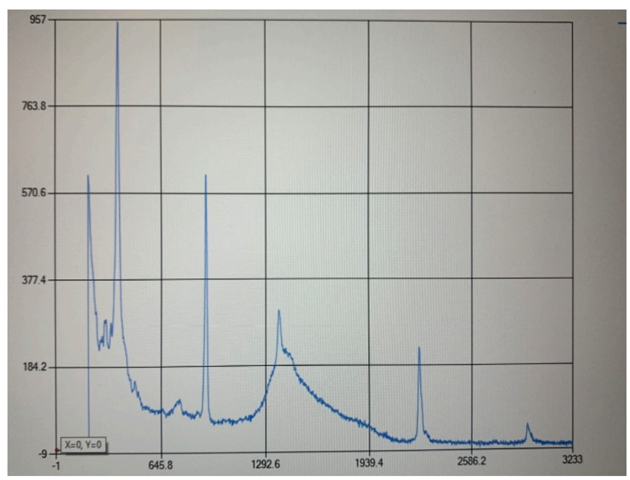
Spectra 1 is a 2-butanone aliphatic ketone that has a peak around 1715 cm^{-1} and peak around 800-700 cm^{-1}, as shown our peak at 763 cm^{-1}. Also, peak at 1400 cm^{-1} our peak at 1418 cm^{-1} has signified the ketone functional group as well.

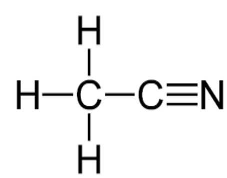




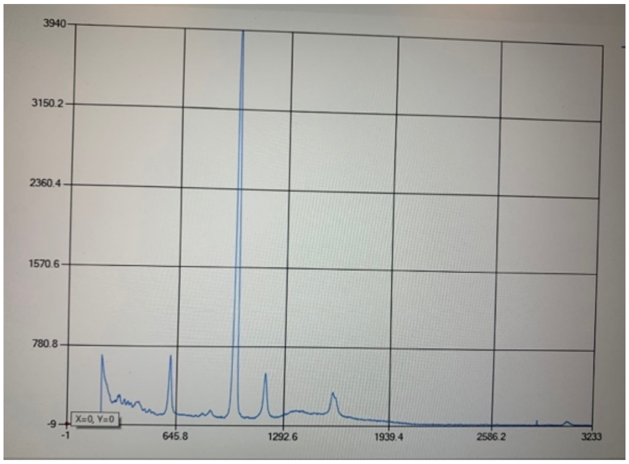
<u>Spectra 1</u>: 2-Butanone,

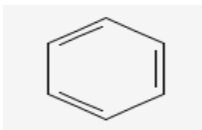
Spectra 2 is acetonitrile and has the C triple bond N with a nitrile peak signified around 2260-2200 cm^{-1} (nitrile), our nitrile peak at 2254 cm^{-1}. The benzene, spectra 3 has shown peaks at 606 cm^{-1} (CCC deformation in plane vib mode), 993 cm^{-1} (benzene ring-breathing mode), 1,177 cm^{-1} (C-H vib. mode), 1586 cm^{-1}(CCC stretching).





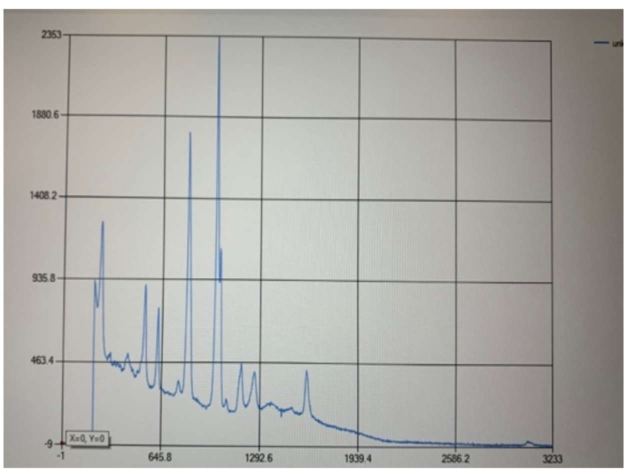
<u>Spectra 2:</u> Acetonitrile,

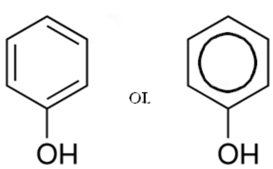




<u>Spectra 3</u>: Benzene,

Spectra 4 signifies a benzene ring with an OH functional group commonly referred to as phenol with peak location 820, 1005, 1255, 1600 cm^{-1}. Note that with the phenol which has similar structure to the Benzene ring structure but the OH functional group bonded to the benzene ring has changed peak locations and stretching are due to additional functional group.





<u>Spectra 4:</u> Phenol,

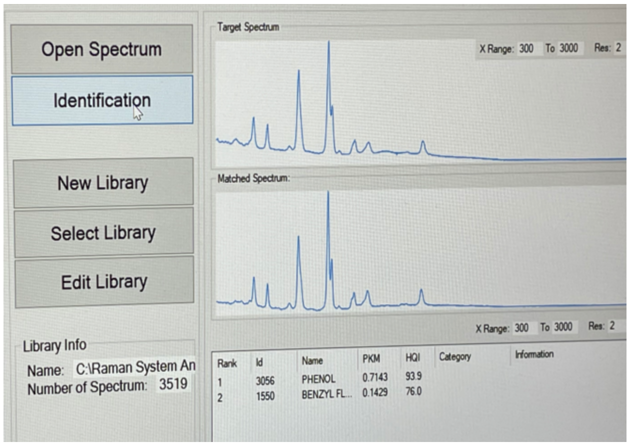
5. CONCLUSION

Since 1930s Raman spectroscopy has been applied to organic systems and is often used in conjunction with IR spectroscopy to give qualitative and structural information. In many cases, Raman spectra are sharp and simple and thus provide advantages over IR in terms of frequency discrimination. Overall there has been abundant deal of progress in bringing Raman spectroscopy to the field, there remain several areas where improvements and further testing are needed. The data system (including the software and library-searching capabilities) will need to improve both in terms of the user interface and the library-search algorithms. A group frequency searching and screening capability would be highly desirable. This capability would provide the responder with an assessment screen that can be used to make educated decisions in the event that the chemical or mixture in question is not in the library. Although not intended to be exhaustive, Table 1 illustrates a few selected compound classes and their characteristic frequency ranges that would be important. There have been continuing research efforts to build chemical libraries for the types of chemicals that the FBI Hazardous Materials Response Unit personnel encounter in the scientific field. An expansion of the library search engine to include frequently encountered mixtures will be a necessity for FBI Hazardous Materials Response Unit applications. Control of the laser power by means of pulsing, beam chopping, or beam spreading may prove necessary as potentially ignitable samples are interrogated. A portable Raman system is needed to discriminate between signal and background light so that shielding will not be required.

Table 1. A Selected List of Warfare Chemicals-FBI materials of interest to analyze

Compound class/substructure	Example(s)	Frequency (cm^{-1})
Chemical warfare agents (methyl phosphonate)	Sarin	685–785
Explosive (nitroaromatic) (nitroester)	TNT, DNT PETN, EGDN, NG	 1310–1390 1260–1300
Propellants/shock sensitive (fulminates) (azides)	Mercury fulminate Lead azide	1250–1350 590–620, 1345–1355

As noted in Table 1, analyzing chemical bonding and learn the different functional groups in Organic Chemistry content are vital for real-world problem solving problems at the FBI. The Raman system will be a valuable front-line screening tool for FBI field investigations. Raman Spectroscopy inquiry lab has allowed our class to study and analyze unknown chemical samples to understand the bonding in more detail. Illustration of various organic chemicals Raman Spectra of unknown samples were analyzed by Raman to better determine the type of bonds/functional groups present. These were all unknown samples that had to be determined by matching the Raman Spectra to the library database, example spectra 5. The phenol in water was studied as well with Raman and found to match the spectra for phenol. Thus, Raman spectroscopy has been found to be feasible to apply it directly to analysis of substances dissolved in water. Therefore, the analysis of rivers, lakes and marine waters without the necessity of prior separations makes Raman spectroscopy advantageous over other analytical instrumentation techniques.



Spectra 5. Phenol with library match

The science educators needed to learn how to analyze and understand organic chemistry bonding and the Raman lab has allowed our students to learn real-world instrumentation. This project has provided the needed knowledge and technological skills for the 21st century for our undergraduate and graduate science education majors at Wright State University (WSU) by providing our students with a Raman Spectroscopy instrument. The **Ohio Learning Standards and Model Curriculum**, K-12, May 2019, and **Next Generation Science Standards (NGSS)** all advocate cooperative, inquiry-based science classroom with technology. However, our WSU students could not realize these national and state goals for science education without skilled, trained K-12 teachers, knowledgeable in interdisciplinary science, pedagogy and technology fields. We have been limited at WSU to train our pre-service/ in-service teachers and general chemistry students with technology such as Raman Spectroscopy. As stated by the standards, "improvements in technology allow us to gather new scientific evidence," but without the updated technology our undergraduate and graduate science education majors could not meet the needed Ohio Department of Education and national science standards. The use of the Raman Spectroscopy instrument was utilized in our Chemistry 3460 –Middle Childhood Education Chemistry class to analyze unknown Organic Chemistry samples. Raman Spectroscopy technique provides detailed information about the chemical structure of the unknown chemical samples which is nondestructive to the samples as well. This is a light scattering technique where a molecule scatters incident light from a high intensity laser light source. A good number of the scattered light occurs at the same wavelength as the laser source thus does not provide useful information which is referred to as Rayleigh Scatter. Typically, 0.0000001% of light is scattered at different wavelengths which depend on chemical structure of the analyte referred to as Raman Scatter. The Raman spectra illustrates a number of peaks where the intensity and wavelength position of the Raman scattered light. Every peak designates to a specific molecular bond vibration such as C-C, C=C, C-H and groups of bonds such as C_6H_6 ring mode, and polymer chain vibrations. The general Raman spectrum provides a unique chemical fingerprint that can be used to identify an unknown chemical sample and a comprehensive Raman spectral library search assists in providing the chemical identification. The Raman spectrum is unique to a material/sample thus it is an excellent technique for identifying/analyzing unknown compounds while allowing students to understand organic chemistry content better. The pre-test and post-test results have shown high content gains utilizing the R.R. Hake' method. Therefore, students have shown an urgent need to understand the chemical bonding and learn the different functional groups in Organic Chemistry content. Raman Spectroscopy inquiry-based lab has allowed our class to study and analyze unknown chemical samples to understand the bonding in more detail. The distinctiveness of the skills outcomes would be: "the learned capacity to think critically, communicate effectively, productively collaborate and perform technical procedures" by P.T. Ewell. Thus, the Raman Spectroscopy instrument has helped our students learn the organic chemistry content and advocate a "broad, rich understanding of novel equipment and its effective use in the role of the world." The pre-test and post-test assessments/outcomes of learning Organic Chemistry content with the use of the Raman Spectroscopy instrument increased content gains greater than 0.70 in content gains understanding organic chemistry bonding, and relating the concept to real-world analysis of hazardous chemicals such as TNT. These hands-on experiences have been found to correlate with increased content gains which are typically found with inquiry-based learning labs (R.R. Hake').

6. REFERENCES

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