AVANTES
MEMBER OF THE NYNOMIC GROUP

EBOOK

SPECTROSCOPY IN RESEARCH

BY AVANTES - EMPOWERING SPECTROSCOPY SOLUTIONS

ABOUT AVANTES

At Avantes, we're not just a company but pioneers in spectroscopy instruments and solutions with almost three decades of experience. We excel in tailoring spectrometer configurations to meet the diverse needs of our customers. We focus on innovation, with the mission is to provide high-quality, customer-oriented optical instruments and solutions.

Our vision extends beyond the lab, aiming to enrich lives and preserve the environment. Avantes instruments and accessories aren't just tools but solutions used globally across various industries. We empower researchers, scientists, and visionaries with cutting-edge spectroscopy technology that transforms how we understand and explore the world.

Our semi-automated manufacturing process further sets us apart, enhancing precision and efficiency while enabling scalable production and exceptional inter-instrument reproducibility. This approach caters to customers ordering large volumes, ensuring our unwavering commitment to outstanding product performance.

Choose Avantes, and join us in shaping the future of analytical science, where precision and innovation meet to illuminate the unknown. Together, we drive discoveries that make a difference.

OUR OFFICES

Avantes Headquarters
Oude Apeldoornseweg 28
7333 NS Apeldoorn
The Netherlands
Telephone: +31 313 670 170
E-mail: info@avantes.com
Website: www.avantes.com

Avantes USA office
2586 Trailridge Dr E, Suite 100
Lafayette, CO 80026
Tel. +1-(303)-410-8668
Phone Toll free: +1 (866)-678-4248
Email: infoUSA@avantes.com
Website: www.avantesusa.com

Avantes China office
Rm.1209-1210, ULO Park,
No.601 Apartment of Wangjing Yuan,
Beijing, 100102 P.R. China
Phone: +86-10-84574045/84574057
Email: info@avantes.com.cn
Website: www.avantes.cn

TABLE OF CONTENT

INTRODUCTION

SPECTROSCOPY IN SCIENTIFIC RESEARCH

Spectroscopy is an essential tool in scientific research, offering precise insights into the composition, structure, and properties of matter through the interaction of light with materials. Whether through absorption, transmission, or scattering, spectroscopy enables researchers to identify substances, analyze their molecular structure, and monitor dynamic processes across a wide range of fields. From environmental monitoring to biomedical diagnostics, the versatility of spectroscopy has made it indispensable in advancing both fundamental science and applied research.

Avantes has been a leader in the field of spectroscopy for over two decades, offering cutting-edge spectroscopic solutions that empower researchers and industries alike. With a portfolio that spans high-performance spectrometers, light sources, and optical components, Avantes supports a broad range of applications—from precise measurements in the life sciences to quality control in industrial processes. Through innovation and expertise, Avantes enables scientists and engineers to push the boundaries of discovery and enhance efficiency in industrial settings.

The purpose of this ebook is to explore how spectroscopy is driving innovating research across multiple scientific and industrial markets. By delving into variuos applications in medicine, agriculture, material science, and beyond, we aim to provide inspiration on how spectroscopic technologies are unlocking new opportunities for research and industry alike. Whether it's enabling faster diagnostics, optimizing environmental monitoring, or ensuring quality control in semiconductor manufacturing, spectroscopy is a cornerstone of progress in today's most critical sectors.

So get ready to dive into various markets and application examples to see how spectroscopy drives innovation forward and get inspired!

1

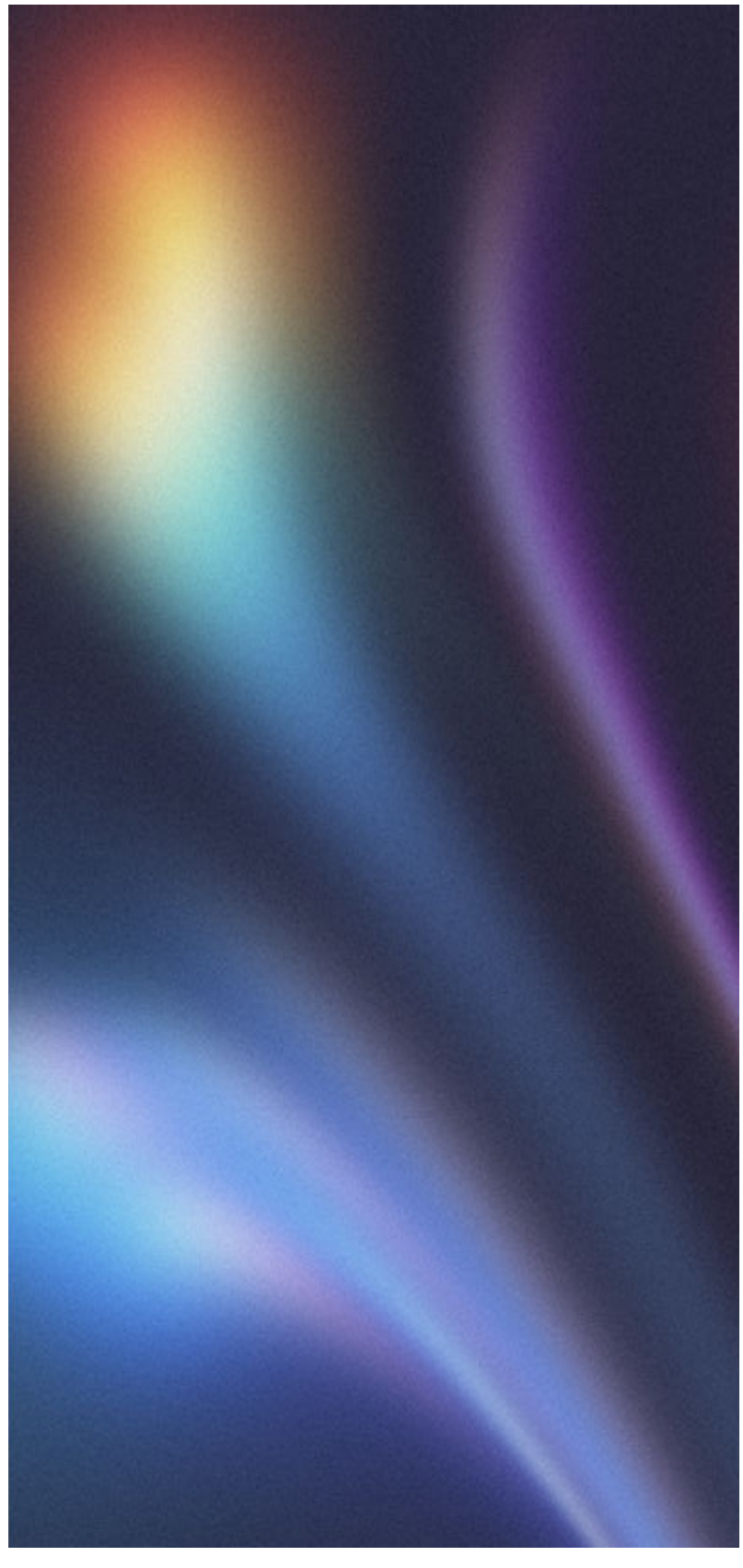
CHAPTER 1

EXPLORATION OF SPECTROSCOPY

1.1 Spectroscopy; the Basics

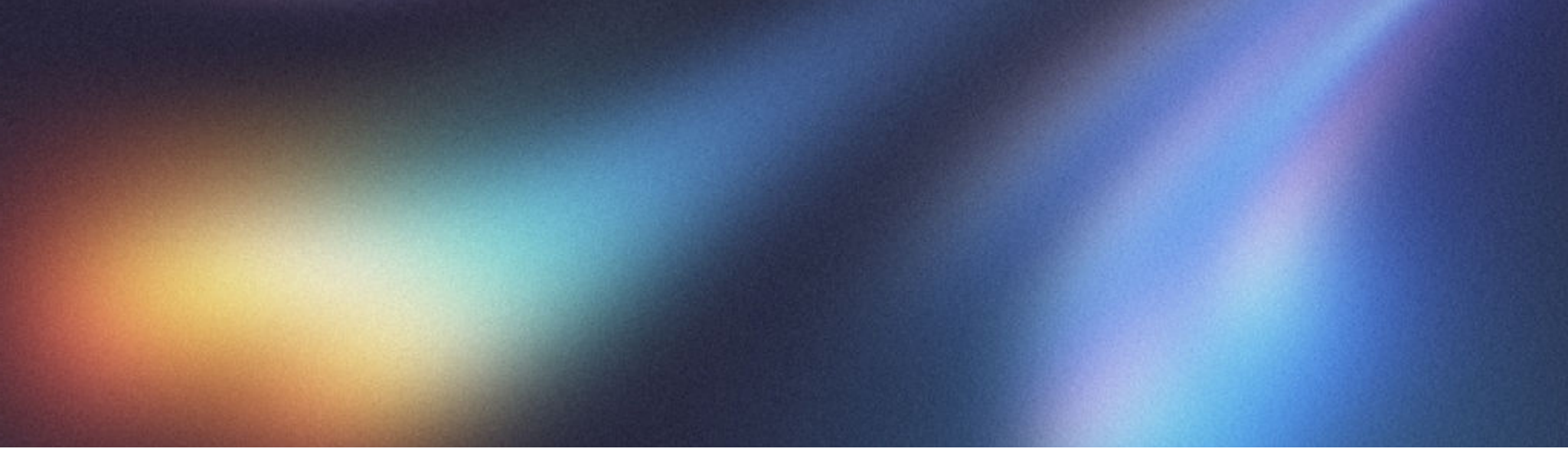
Spectroscopy is the study of the interaction between light (electromagnetic radiation) and matter. By analyzing how materials absorb, emit, or scatter light across different wavelengths, researchers can gain valuable insights into the composition, structure, and properties of a substance. Spectroscopy can be applied to solids, liquids, gases, and even biological tissues, making it a versatile and essential tool across many scientific disciplines.

At its core, spectroscopy exploits the fact that different molecules and atoms interact with light in characteristic ways. These interactions create unique spectral signatures that can be used to identify materials and observe changes at the molecular or atomic level. Whether studying the properties of new materials, investigating biological samples, or monitoring chemical reactions, spectroscopy provides a window into the molecular world that is both precise and non-invasive.



1.2 Common Types of Fiber Optic Spectroscopy

Over the years, several types of spectroscopy have been developed to study different aspects of matter. Each method has its strengths and specific applications in research, with some of the most widely used techniques being UV-Vis spectroscopy, NIR spectroscopy, and Raman spectroscopy.



1.2 Common Types of Spectroscopy

UV-Visible (UV-Vis) Spectroscopy

UV-Vis spectroscopy measures the absorption or reflectance of ultraviolet and visible light by a sample. It is commonly used in chemistry, biology, and environmental science to analyze the concentration of substances, detect impurities, and monitor chemical reactions. For instance, in biochemical research, UV-Vis spectroscopy helps quantify nucleic acids and proteins, providing insights into their concentrations and purity. Additionally, environmental scientists use UV-Vis spectroscopy to monitor water quality by detecting contaminants like nitrate or phosphate.
Click the blue words to read more information about the measurement techniques absorption and reflection.

Near-Infrared (NIR) Spectroscopy

NIR spectroscopy focuses on the near-infrared region of the electromagnetic spectrum and is particularly effective for analyzing organic compounds and biological tissues. It has found widespread use in agriculture, food science, and medicine due to its ability to penetrate deeply into samples and provide real-time analysis. In agriculture, NIR spectroscopy is employed to assess crop health, soil composition, and the nutritional content of food products.
In the medical field, NIR is valuable for non-invasive monitoring of tissues, offering real-time data on oxygen levels, blood flow, and metabolic activity.

Raman Spectroscopy

Raman spectroscopy is a technique that analyzes how light scatters after interacting with the vibrational modes of molecules. It provides detailed information about molecular structures and is particularly useful for studying complex biological materials, nanomaterials, and chemical compounds. In pharmaceutical research, Raman spectroscopy aids in drug development by characterizing molecular compounds and monitoring chemical processes. Its ability to provide non-invasive, high-resolution data makes it an invaluable tool in fields like forensic science and material science, where precise identification of compounds is crucial. Click here to read more information about Raman spectrsocopy.

1.3 Advantages of Spectroscopy

Spectroscopy offers several unique advantages that make it indispensable in modern research. One of the key benefits is its **non-invasive nature**. Many spectroscopic techniques, such as NIR and Raman, allow researchers to analyze samples without the need for complex preparation or destructive testing. This is especially important in fields like medicine and environmental science, where preserving the integrity of a sample is critical.

Another major advantage of spectroscopy is its ability to provide **real-time data.** Spectroscopic techniques can often monitor dynamic processes as they happen, such as chemical reactions, metabolic changes in living tissues, or material stress during manufacturing. This capability to track changes in real time helps researchers gain a deeper understanding of the mechanisms at play in their experiments or industrial processes.

Finally, spectroscopy is known for its **precision and accuracy.** The ability to measure specific wavelengths and their interaction with matter enables researchers to detect even minute changes in molecular composition or structure. This level of detail is invaluable in applications ranging from quality control in industrial production to advanced medical diagnostics.

1.4 Conclusion

In summary, spectroscopy stands out as a critical tool in scientific research due to its ability to provide accurate, non-invasive, and real-time data across a variety of fields. From the detection of pollutants in environmental studies to the characterization of new materials and the monitoring of complex biological processes, spectroscopy continues to drive innovation and discovery.

In the chapters that follow, we will explore how spectroscopy is applied in key markets, highlighting its transformative impact in fields like medicine, agriculture, material science, and industrial control. You can expect to read interesting application notes, experiments and product highlights.

If you, at any point, have questions about the content or products, feel free to reach out to our support engineers through our website, by clicking here.

2

CHAPTER 2

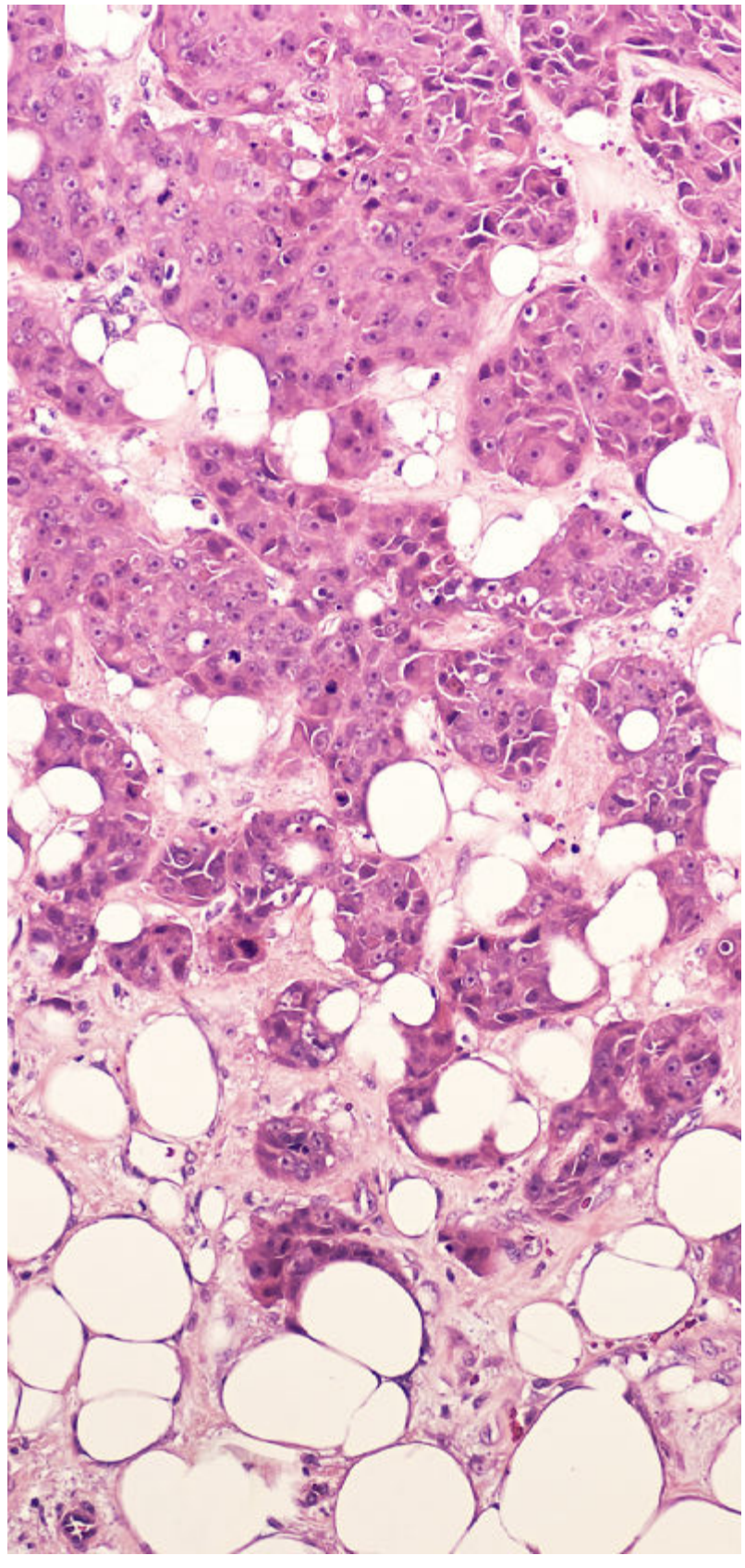
(BIO)MEDICAL & MEDICINE SCIENCES

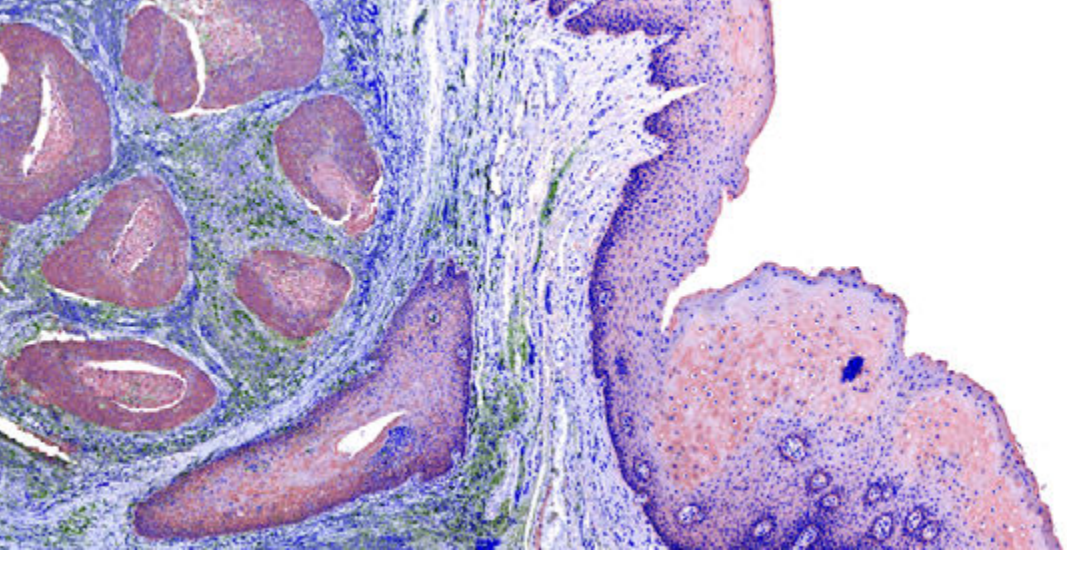
2.1 Introduction Spectroscopy in (Bio)Medical & Medicine Sciences

Spectroscopy has established itself as an indispensable tool in biomedical, medical, and life sciences research. It enables researchers to explore biological systems at the molecular level, offering insights into the biochemical and structural properties of tissues, cells, and fluids. What makes spectroscopy particularly valuable in these fields is its ability to provide non-invasive, real-time data, making it ideal for studying living organisms without disrupting their natural state.

In biomedical research, spectroscopy supports the development of diagnostic tools and the study of disease mechanisms. Techniques such as near-infrared (NIR) and Raman spectroscopy allow scientists to identify molecular biomarkers, detect diseases at early stages, and even monitor the progression of conditions like cancer and cardiovascular disease. In medicine, spectroscopic technologies are revolutionizing areas like imaging, pharmaceutical development, and personalized therapies by offering precise molecular insights.

In this chapter, we will dive into how spectroscopy is applied across these vital fields, examining specific applications and research studies that highlight its transformative impact.





2.2 Application Notes

2.2.1 ELEVATING TISSUE IDENTIFICATION WITH SPECTROSCOPY

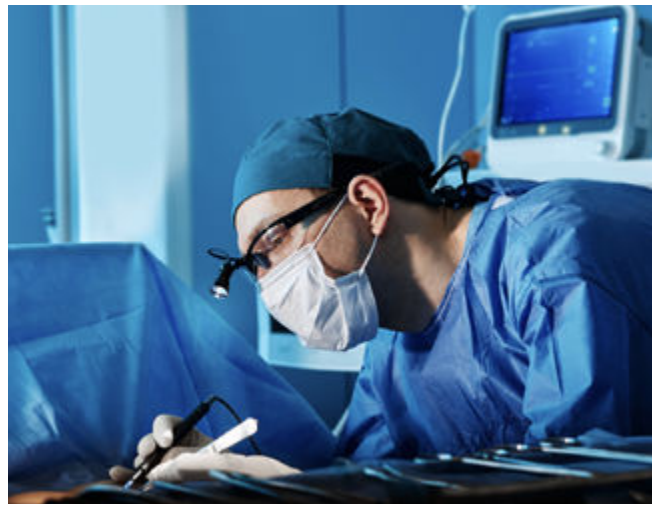
Tissue identification is a crucial part of any medical process. Disease diagnosis, making surgical decisions, and treatment plans – all of these steps benefit from advanced tissue identification techniques. In conventional medical diagnostics, the procedure typically involves obtaining a biopsy sample from the patient, followed by meticulous analysis, often utilizing microscopy techniques within a laboratory setting. While histopathology is often regarded as the 'gold standard' for cancer diagnosis,[1] it is not without limitations. The invasive nature of biopsy sampling poses discomfort for patients, the precision of the sampling process impacts diagnostic accuracy,[2] and the urgency of clinical decision-making necessitates efficient procedures for optimal patient outcomes.[3] This article will explore the challenges posed by traditional tissue identification methods and identify emerging technologies and approaches that promise to revolutionize this critical aspect of medical practice.

THE ADDED VALUE OF SPECTROSCOPY IN TISSUE IDENTIFICATION

Spectroscopic techniques are already used in laboratory and clinical settings for successfully diagnosing cancers and tissue discrimination.[4-7] What makes spectroscopic tissue analysis so invaluable is the chemical information the spectroscopic technique can retrieve. Unlike relying on visual cues in imaging microscopy, spectroscopic methods capitalize on detecting specific chemical biomarkers present in tissues. This nuanced approach also further enhances the accuracy of tissue identification and characterization.[5] One of the key advantages of using spectroscopic methods, particularly with longer wavelength radiation, is that the radiation has an improved penetration depth and can be used to visualize tissue structures inside the body without the need for surgery. This way, vital information regarding the location, depth, and composition of tissue structures can be obtained, all while ensuring minimal discomfort to the patient.

REAL-TIME DIAGNOSTICS

In addition to bolstering diagnostic precision, cutting-edge spectrometers like the Avantes series can provide real-time imaging information even during a surgical process. The Avantes AvaSpec-VARIUS or HS2048XL, when paired with an Avantes light source or combined with fiber optic probes, proves instrumental in distinguishing between human tissue and prosthetics. Leveraging the advantages of both reflectance and transmission modes, these instruments enable surgeons to discern subtle variations in tissue composition, aiding in surgery navigation and ensuring optimal patient outcomes.



SPECIFIC APPLICATIONS FOR SPECTROSCOPY

Spectrometers play a pivotal role in various medical diagnostic applications, showcasing their versatility and precision, some of which are outlined below:

Smart Biopsy for Oncological Precision

Spectrometers introduce the concept of the 'smart biopsy,' leveraging real-time analysis capabilities to address challenges in oncology, particularly in ensuring complete tumor removal.[8] By integrating spectroscopic capabilities into surgical tools, such as the surgical knife, surgeons gain access to a 'smart' tool capable of discriminating between tissue types in real-time through reflectance measurements. This advancement enhances the precision of biopsies and mitigates the risk of missing cancerous regions.

Enhancing Precision in Anesthesia Delivery

The high spatial resolution of spectroscopic techniques extends beyond biopsy procedures to other high-precision interventions, including anesthesia delivery.[9] Incorporating fiber optics and spectroscopy into the needle tip revolutionizes anesthesia administration, particularly regional anesthesia. By discriminating nerve tissue from its surroundings in real-time, spectrometerequipped needles ensure accurate and effective nerve blocks, minimizing the risk of nerve damage and enhancing patient safety.[9]

Accurate Depth Determination for Targeted Treatments

Spectroscopic information can also provide accurate depth determination, crucial for various medical interventions. Depth information proves invaluable in locating tissues like nerves and optimizing treatment doses, as exemplified in radiotherapy. By precisely determining tissue depth, spectrometers contribute to dose minimization strategies, reducing unwanted side effects and improving patient outcomes.[10]

FUTURE FRONTIERS IN TISSUE IDENTIFICATION

Integrating spectroscopic techniques into tissue identification has already revolutionized the quality of medical information available to clinicians, leading to improved diagnosis times and the acquisition of novel insights during surgical procedures. Spectroscopic methods offer the advantage of non-invasiveness, mitigating clinical risks associated with traditional diagnostic procedures. As a result, invasive surgical biopsies may soon be replaced by minimally invasive techniques similar to pulse oximetry.

The development of compact, hand-held spectrometers also opens many possibilities for point-of-care diagnostics, extending the reach of advanced diagnosis beyond traditional medical settings. These portable devices offer real-time insights and non-invasive characterization, paving the way for enhanced precision in diagnostics and treatment guidance.

REFERENCES

1. Irshad, H., Member, S., Veillard, A., Roux, L., & Racoceanu, D. (2014). Methods for Nuclei Detection , Segmentation , and Classification in Digital Histopathology : A Review — Current Status and Future Potential. IEEE Reviews in Biomedical Engineering, 7,97–114. https://doi.org/10.1109/RBME.2013.2295804

2. Neal, R. D. (2009). Do diagnostic delays in cancer matter ? British Journal of Cancer, 101, 9-1S2. https://doi.org/10.1038/sj.bjc.6605384

3. Pritzker, K. P. H., & Nieminen, H. J. (2019). Needle Biopsy Adequacy in the Era of Precision Medicine and Value-Based Health Care. Arch Pathol Lab Med, 143, 1399–1415. https://doi.org/10.5858/arpa.2018-0463-RA

4. Blondel, W., & Delconte, A. (2021). Diffuse Reflectance Spectroscopy : SpectroLive Medical Device for Skin In Vivo Optical Biopsy. Electronics, 10, 243.

5. Santos, I. P., Barroso, E. M., Schut, C. B., Caspers, P. J., Lanschot, C. G. F. Van, Choi, D., & Kamp, M. F. Van Der. (2017). Raman spectroscopy for cancer detection and cancer surgery guidance : translation to the clinics. Analyst, 142, 3025–3047. https://doi.org/10.1039/c7an00957g

6. Amani, M., Bavali, A., & Parvin, P. (2022). Optical characterization of the liver tissue affected by fibrolamellar hepatocellular carcinoma based on internal filters of laser - induced fluorescence. Scientific Reports, 1–10. https://doi.org/10.1038/s41598-022-10146-7

7. Hendriks, B. H. W., Balthasar, A. J. R., Lucassen, G. W., Voort, M. Van Der, Kortsmit, J., Langhout, G. C., & Geffen, G. J. Van. (2015). Nerve detection with optical spectroscopy for regional anesthesia procedures. Journal of Translational Medicine, 1–11. https://doi.org/10.1186/s12967-015-0739-y

8. Amiri, S. A., Dankelman, J., & Hendriks, B. H. W. (2024). Enhancing Intraoperative Tissue Identification : Investigating a Smart Electrosurgical Knife ' s Functionality During Electrosurgery. IEEE Transactions on Biomedical Engineering, PP, 1–12. https://doi.org/10.1109/TBME.2024.3362235

9. Hendriks, B. H. W., Balthasar, A. J. R., Lucassen, G. W., Voort, M. Van Der, Kortsmit, J., Langhout, G. C., & Geffen, G. J. Van. (2015). Nerve detection with optical spectroscopy for regional anesthesia procedures. Journal of Translational Medicine, 1–11. https://doi.org/10.1186/s12967-015-0739-y

10. Naumann, P., Batista, V., Farnia, B., & Fischer, J. (2020). Feasibility of Optical Surface-Guidance for Position Verification and Monitoring of Stereotactic Body Radiotherapy in. Frontiers in Oncology, 10, 573279. https://doi.org/10.3389/fonc.2020.573279

2.2.2 INDOCYANINE GREEN (ICG) FLUORESCENCE - RAMAN ANALYSIS

Indocyanine Green (ICG) is a powdered dye used for fluorescence imaging in various medical applications. ICG emits fluorescence between 750 nm and 950 nm with maximum values of approximately 810 nm when dissolved in water. Compared to other fluorescence imaging dyes, ICG provides imaging in the Near-Infrared (NIR) range from 780 nm to 2500 nm. The NIR range offers deeper imaging that operates in the tissue optical window. The tissue optical window ranges from 650 nm to 1350 nm, the range where light has a maximum depth to penetrate tissue. For medical applications, ICG powder is dissolved in sterile water, preparing the solution for injection. The injection solutions are highly concentrated, but differ based on the application. Some of the uses for ICG consist of hepatic function studies (preparative tests for major liver surgery), ophthalmic angiograms (tests on blood vessels and other structures in the back of the eye), and lymphatic mapping (lymph nodes, lymphatic vessels, and lymphatic fluid). The ICG injection solution is paired with an infrared laparoscope in surgical applications. The fluorescence light passes through the laparoscope's optical filter, allowing surgeons to work in two different infrared modes. The first IR mode detects detailed structures under infrared light. The second IR mode shows the pure fluorescence with the highest contrast in a black-and-white image. The ICG absorbs the infrared radiation from the light source and emits longer wavelengths of infrared radiation, which makes ICG detectable in the human body.

In this experiment, concentrations were made in the 2 to 50 micromolar range. A micromolar is a concentration of one-millionth molecular weight per liter. This range allows light to pass through the solution without fully absorbing it. If tests were conducted with the surgical application concentrations, the deep, dark green color of the ICG would absorb most, if not all, of the light. Usually, the more concentrated a dye, the more fluorescence it will emit. However, a highly concentrated solution of ICG is almost black, making it optical opaque and unsuitable for a fluorescence reading. Upon observing this, Dr. John Black, a chair for IEEE Engineering in Medicine & Biology Society was contactedm and he recommended the range of 2 to 50 micromolar.

USED SYSTEM

For this experiment, we used the AvaSpec-HERO spectrometer. The AvaSpec-HERO is built up around our High-Sensitivity, Compact (HSC), 100mm optical bench offering a NA of 0.13 and a cooled, back-thinned detector (1024×58 pixels). Electronics-wise, it uses our latest AS7010 board, which includes a high-performance Analog to Digital converter with excellent signal-to-noise performance and the ability to facilitate high-speed communication through USB 3.0 and Ethernet.
Due to this instrument's high sensitivity and signal-to-noise, the HERO is ideal for fluorescence measurements.

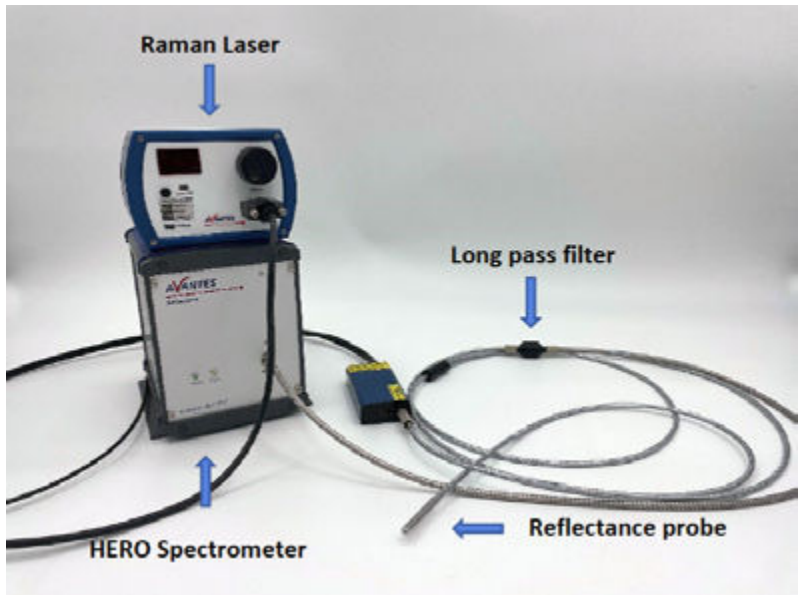


FIGURE 1: Setup of Fluorescent Test

To excite the sample, a 785 nm Raman laser was used. The laser is attached in line to a reflection probe. On the receiving end of the reflection probe, a long pass filter was used to block the 785 nm laser from being seen by the spectrometer (Figure 1). This ensured that the user observed only the fluorescence emission peak.

DESCRIPTION OF METHODOLOGY

The first step taken in was determining the proper solution concentrations. The range that would be best to test the fluorescence of ICG was recommended to be 2 to 50 micromolar. In the first tests we ran before consulting with Dr. John Black, we used surgical concentrations of 1.25 mg/mL, 5 mg/mL, and 20 mg/mL. These concentrations corresponded to different medical applications, respectively. The injection solution of 1.25 mg/mL is used for lymphatic mapping, the injection solution of 5 mg/mL is for hepatic function studies, and the injection solution of 20 mg/mL is used for ophthalmic angiograms. After running a couple of tests using these concentrations, we realized that the solutions were too dark in color for proper fluorescence readings. Although these concentrations are used in surgical procedures with laparoscopic equipment and receive proper readings, the higher concentrated solutions have a different host material than we were experimenting with. ICG responds differently to respective host materials. In this experiment, we used distilled water as our solvent. We converted the micromolar values to mg per mL to get the proper concentrations in the micromolar range. We evenly split up nine groups among the range and found the theoretical concentrations in mg/mL using dimensional analysis and Excel (Figure 2). To be able to carry out the theoretical concentrations, base concentrations were made of the ICG and distilled water (Figure 3).

					Theoretical
Tests	Micromolar (μM)	Molar (mol/L)	(L/mol)	(g/L)	Concentrations (mg/mL)
1	2	0.000002	500000	0.00155	0.00155
2	8	0.000008	125000	0.0062	0.0062
3	14	0.000014	71428.571	0.01085	0.01085
4	20	0.00002	50000	0.0155	0.0155
5	26	0.000026	38461.538	0.02015	0.02015
6	32	0.000032	31250	0.0248	0.0248
7	38	0.000038	26315.789	0.02945	0.02945
8	44	0.000044	22727.273	0.0341	0.0341
9	50	0.00005	20000	0.03875	0.03875

FIGURE 2: Converting micromolar to mg per mL

Base Concentrartions	(mg/ml)	ICG (mg)
1	0.050	0.050
2	0.10	0.10
3	0.20	0.20

FIGURE 3: Base concentrations in distilled water

The base concentrations were then diluted with more distilled water to get the concentrations that were needed in the proper range (Figure 4). The highlighted yellow values used the first base concentration of 0.050 (mg/mL), the light green used the second base concentration of 0.10 (mg/mL), and the dark green values used the third base concentration of 0.20 (mg/mL). One milliliter of base concentration was added to the highlighted values to get the wanted concentration. More calculations were then run to find the actual concentrations based on the amount of sensitivity we have with our equipment. The actual concentrations were then converted back to micromolar to see a more accurate range of the concentrations made (Figure 4). The final nine concentrations can be seen in Figure 5.

		Add this		Check	Actual			Actual
ICG/ Conc (mL)	Added DW	Scaled (mL)	ICG/ Conc	Concentrations	Scaled (mg/mL)	(L/mol)	Molar (mol/L)	Micromolar (μM)
32.25806452	31.258065	31	32.0	0.0015625	0.0016	484375	2.1E-06	2.1
8.064516129	7.0645161	7.0	8.0	0.00625	0.0063	123016	8.1E-06	8.1
9.216589862	8.2165899	8.0	9.0	0.011111111	0.011	70454.5	1.4E-05	14.2
6.451612903	5.4516129	5.5	6.5	0.015384615	0.015	51666.7	1.9E-05	19.4
4.962779156	3.9627792	4.0	5.0	0.02	0.020	38750	2.6E-05	25.8
8.064516129	7.0645161	7.0	8.0	0.025	0.025	31000	3.2E-05	32.3
6.791171477	5.7911715	6.0	7.0	0.028571429	0.029	26724.1	3.7E-05	37.4
5.865102639	4.8651026	5.0	6.0	0.033333333	0.033	23484.8	4.3E-05	42.6
5.161290323	4.1612903	4.0	5.0	0.04	0.040	19375	5.2E-05	51.6

FIGURE 4: Calculations of actual concentrations and micromolar range from theoretical values

FIGURE 5: Different concentrations of ICG with distilled water

We first ran the experiment in a fully lit room. We soon realized that the equipment was picking up the ambient light in the room due to the low concentrated solutions. So we ran the tests in a blackout room. The spectra no longer had ambient light influences, and the fluorescence of ICG could be analyzed. We measured the spectra from the samples by submerging the reflectance probe in each vial. The probe held steady for around 30 seconds or until a solid reading was received. The integration time was for 3 seconds with an average of 2. The reflection probe was cleaned with distilled water and wiped down between each reading.

TEST DATA & RESULTS

Figures 6-15 show the experimental results from the ICG fluorescence measurements. For this experiment's raw scope, A/D counts from the spectrometer are used rather than calibrated fluorescence counts coming from a radiometric calibration of the spectrometer's sensitivity. A possible future variant of this experiment would include re-measurement with a radiometrically calibrated spectrometer.

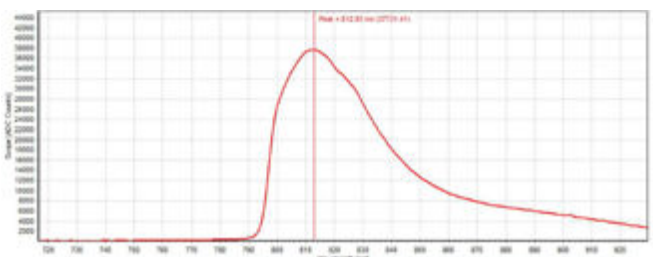


FIGURE 6: Sample 1: 0.0016 mg/mL concentration (2.1 µM)

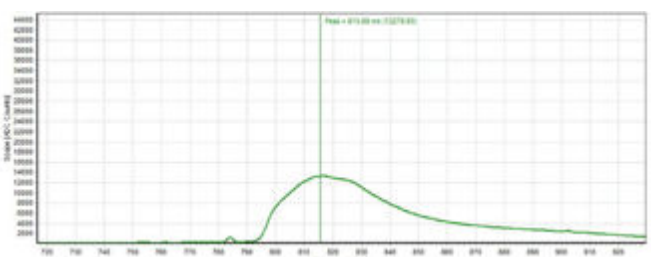


FIGURE 7: Sample 2: 0.0063 mg/mL concentration (8.1 µM)

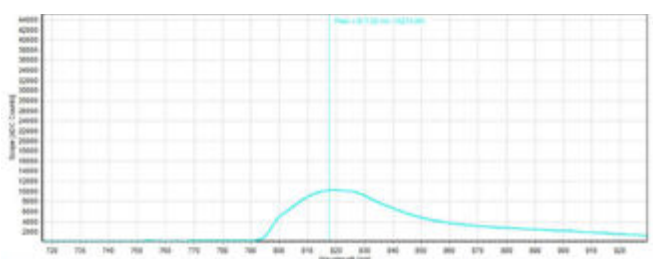


FIGURE 8: Sample 3: 0.011 mg/mL concentration (14.2 µM)

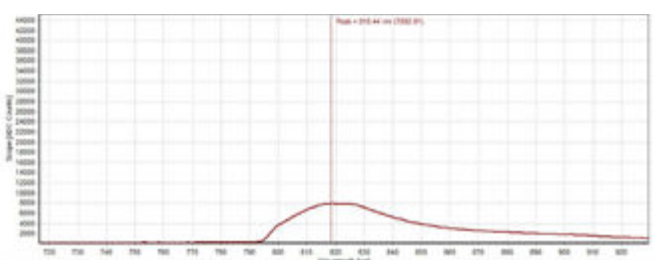


FIGURE 9: Sample 4: 0.015 mg/mL concentration (19.4µM)

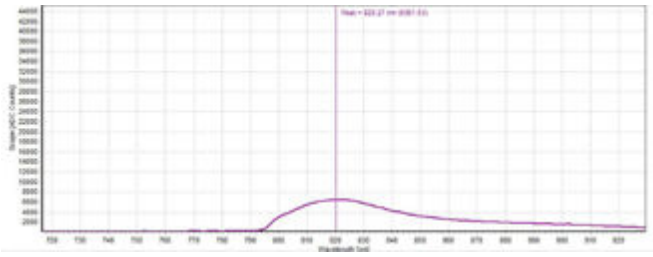


FIGURE 10: Sample 5: 0.020 mg/mL concentration (25.8 µM)

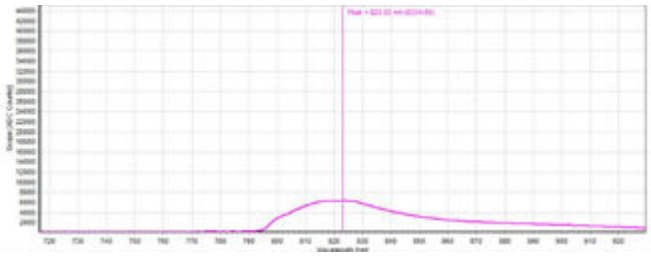


FIGURE 11: Sample 6: 0.025 mg/mL concentration (32.3 µM)

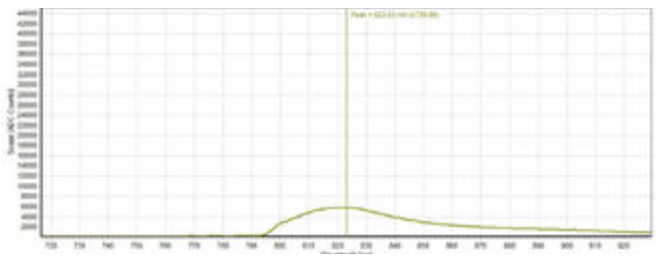


FIGURE 12: Sample 7: 0.029 mg/mL concentration (37.4 µM)

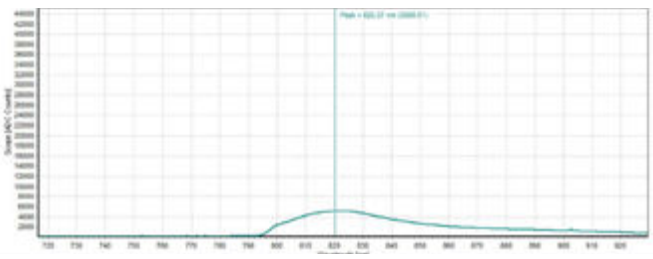


FIGURE 13: Sample 8: 0.033 mg/mL concentration (42.6 µM)

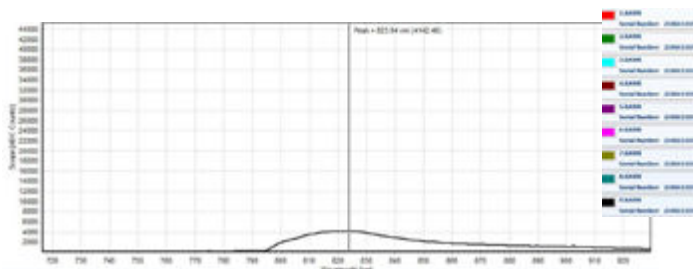


FIGURE 14: Sample 9: 0.040 mg/mL concentration (51.6 µM)

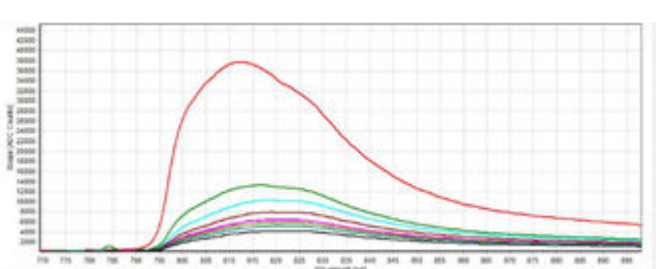


FIGURE 15: Spectra of the nine concentrations

ANALYSIS & CONCLUSION

From the spectra received, the trend of fluorescence peaks shows that the more concentrated samples had shallower fluorescence spectrums but higher max peaks. For example, sample 1 (Figure 6) had a concentration of 0.0016 mg/mL with the largest spectrum and had a max peak of 812.93 nm. Sample 2 (Figure 7) had a concentration of 0.0063 mg/mL with the second-largest spectrum and had a max peak of 815.68 nm. This pattern continued fairly consistently with all of the samples. ICG emits fluorescence between 750 nm and 950 nm with maximum values of approximately 810 nm when dissolved in water. The sample's maximum peak values ranged from 812.93 nm to 823.94 nm. The spectra obtained matched the literature describing fluorescence emission.

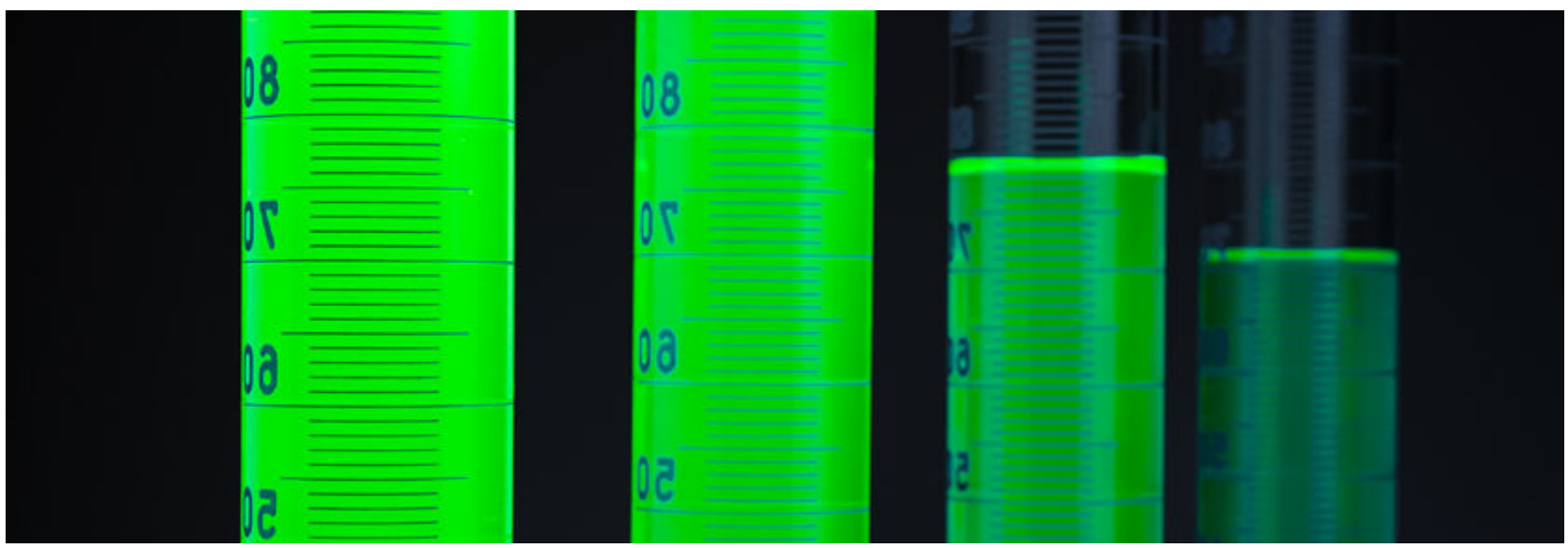
Usually, the more concentrated a dye, the more fluorescence it emits. However, in this case, ICG does the exact opposite. ICG has special properties that could be the cause of this. For starters, ICG has close excitation and emission spectra that often leads to the excitation light being detected together with the emission signal. ICG has an excitation emission at around 790 nm. The overlap of spectra exhibits concentration-dependent fluorescence quenching. Quenching refers to any process that lowers the fluorescence intensity. Excited-state reactions, energy transfer, and formational collisions can all result in quenching. Dr. Black, with the Medicine and Biology Society, described this phenomenon by adding that ICG's molecules are close enough to self-absorb the fluorescence photons and convert this energy into vibration (heat) by some internal conversion mechanism.

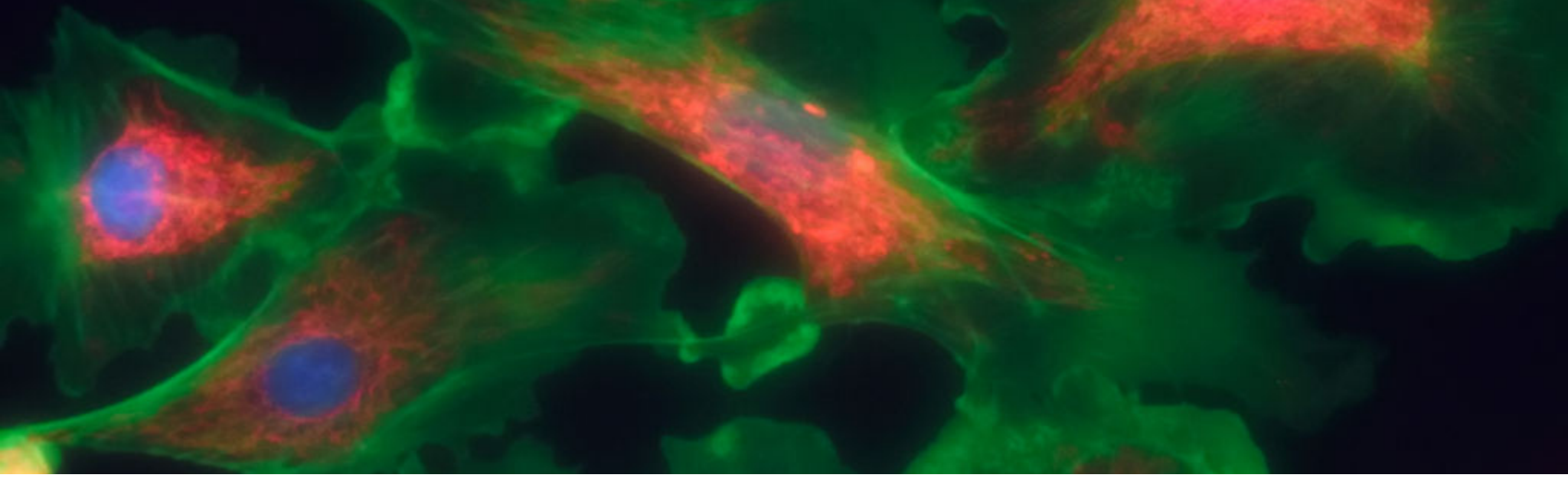
The explanation of the ICG fluorescence trend is not entirely known. ICG has been notorious for receiving interesting and non-linear readings. The chemical and spectroscopic properties of ICG can cause quenching of solutions. However, in medical applications, the same trend does not always follow. ICG, when injected into a human body, responds very differently than when tested with distilled water with no other host material. In some applications, ICG cannot be read at any concentration. Some of the host materials with the best medical implant properties cannot read the ICG. Similar to when we ran the ICG solutions with the higher concentrations, some host materials create an almost black coloring that absorbs all the light and does not allow for a proper reading.

CONCLUSION:

Indocyanine Green and fluorescence imaging testing is beneficial to many medical applications. The powdered green dye reaches the Near-Infrared range (NIR), which offers deeper imaging in the tissue optical window. ICG is non-toxic, inexpensive, and relatively easy to use in medical applications. It is an excellent asset to fluorescence testing and is currently the most popular imaging mode. With all this said, ICG remains to be tested and tried. A lot of its properties, especially pertaining to fluorescence, is unknown and cannot be explained in full. After conducting this experiment, we validated some key factors of ICG fluorescence testing:

1. The concentration of the ICG is important. Based on the solvent and/or host material, the concentration needs to be calculated correctly, or the instrumentation will not be able to read the spectra.
2. The setup of the system needs to block out the excitation-emission. In this experiment, we used a 785 nm Raman laser light source and a long pass filter to ensure that the excitation-emission did not overly interfere with the fluorescence emission.
3. With the low concentration samples, a darkroom was required for testing so that the reflectance probe would not pick up ambient light.





2.2.3 MORE APPLICATION NOTES

If you're interested in exploring more in-depth research and applications of spectroscopy in medical fields, we invite you to visit our website. There, you'll find a wide range of case studies and detailed insights into how spectroscopy is advancing innovations in diagnostics, pharmaceutical testing, tissue analysis, and much more. Whether you're focused on medical research, clinical applications, or life sciences, our extensive library of application notes can provide valuable information to support your work. Explore more here.

2.3 Key Takeaways BioMedical & Medicine Sciences

Spectroscopy has become an essential tool in biomedical and medical research, offering unparalleled insights at the molecular level. Its non-invasive, real-time capabilities make it indispensable for studying living organisms and developing precise diagnostic tools. Techniques like near-infrared (NIR) and Raman spectroscopy enable early detection of diseases by identifying molecular biomarkers, helping researchers track disease progression, and offering personalized treatment options. These techniques allow for dynamic monitoring without disrupting biological systems, making them ideal for both laboratory research and clinical settings.

Fiber-optic spectrometers, in particular, stand out for their ability to facilitate in-situ (in vivo) measurements in clinical environments. This technology is widely used in various applications, such as blood analysis, tissue fluorescence, and phototherapy.

It is especially valued for its affordability, enabling low-cost, disposable testing devices that improve the accessibility and efficiency of medical diagnostics. Furthermore, spectroscopy's role in pharmaceutical testing ensures that new drugs meet strict safety and quality standards, streamlining the path from research to patient care.

Avantes has played a pivotal role in advancing spectroscopy solutions for both researchers and Original Equipment Manufacturers (OEM). By offering flexible, cost-effective, and precise spectroscopic instruments, Avantes continues to support innovations in medicine and life sciences. For further exploration of our case studies and real-world applications, we invite you to visit our website, or contact our technical engineers for more information about our products, capabilities, and more.

3

CHAPTER 3

ENVIRONMENTAL, AGRICULTURE & FOOD SCIENCES

3.1 Introduction Spectroscopy in Environmental, Agriculture & Food Sciences

Spectroscopy plays a crucial role in environmental, agricultural, & food sciences by enabling precise analysis of various materials. Spectroscopy offers non-invasive, real-time measurements, making it an ideal tool for monitoring ecosystems, assessing soil and crop health, and ensuring food quality. Its versatility and accuracy make it indispensable for researchers tackling pressing global challenges.

In **environmental science**, spectroscopy is widely used to monitor air and water quality, detect pollutants, and study soil composition. Techniques like UV-Vis provide detailed information about contaminants and nutrient levels, helping scientists assess ecosystem health and track the effects of pollution over time. In **agriculture**, spectroscopy aids in optimizing crop yields and improving soil management. NIR spectroscopy is used to analyze moisture levels, monitor plant health, and assess nutrient content in soil. These insights help farmers adopt more sustainable practices and respond to changing environmental conditions more effectively. Similarly, in **food science**, spectroscopy ensures the quality and safety of products by detecting contaminants, verifying authenticity, and analyzing nutritional content. Through applications like these, spectroscopy supports innovation across the entire food supply chain, from farm to table.

In this chapter, we explore a few application examples that demonstrate spectroscopy's role in these vital fields.

3.2 Application Notes

3.2.1 SPECTROSCOPY IN ENVIRONMENTAL SCIENCES

As industries of all sorts advance throughout the global marketplace, both the need for ecological monitoring and the technology to implement it, advance as well. Several spectroscopic measurement techniques are proving to be effective and versatile for environmental applications. Fluorescence measurements are a typical choice for detecting the presence of hydrocarbon pollutants, while Raman spectroscopy might be used to identify organic contaminants. Laser-induced breakdown spectroscopy (LIBS) and fluorescence measurements are both used in processing nuclear material, and we see absorbance spectroscopy used in water quality monitoring of coastal waterways. The need for environmental and ecological testing and measurement is constantly on the rise and there are a number of spectroscopy methods available.

APPLICATION EXAMPLE: SPECTROSCOPY IN WATER CONTAMINATION MONITORING

Monitoring water quality is crucial for protecting human health, aquatic ecosystems, and overall environmental sustainability. Contaminated water can lead to serious health , and environmental risks. Real-time monitoring of water quality is essential for prompt response to pollution events and for ensuring compliance with environmental regulations.

Spectroscopy has significant advantages over conventional water monitoring techniques, such as colorimetric methods and titration, which can be time-consuming and labor-intensive. Traditional methods often require sample preparation and chemical reagents, leading to longer turnaround times and increased costs. Spectroscopy provides rapid, non-invasive analysis, allowing for immediate results and on-site assessments. Techniques like UV-Vis spectroscopy can detect a wide range of contaminants, including heavy metals, pesticides, and organic pollutants, with high sensitivity and specificity.

DETECT LOW LIMITS OF PARTICLES IN WATER

Absorbance spectroscopy can bring entirely new perspectives on samples through a wide range of industries. This includes the water industry, verifying the quality and purity of water to determine what contaminants and particles may be present in the water, that may not be visible to the human eye.

Being able to detect low limits of particles in water is extremely crucial, therefore a highly sensitive spectrometer is needed to detect parts per million (ppm). In this experiment, we show you the power of Avantes solutions to detect these low concentrations.

USED SYSTEMS & METHODOLOGY

The setup for this experiment utilizing an AvaSpec-HERO, coupled to a path cuvette holder and AvaLight-DH-S-BAL light source to measure the absorbance through the sample.

The AvaSpec-HERO is a top-of-the-line spectrometer. Based on our High Sensitivity Compact (HSC) optical bench (f=100mm; NA=0.13) and a 1024×58 back-thinned CCD detector, it offers the best of both worlds: high sensitivity and resolution. The instrument is equipped with thermoelectric cooling, enabling long integration times in low light applications. In conjunction with our AS7010 electronics, including a high-end AD convertor, noise is kept to a minimum, which gives you an excellent Signal to Noise and Dynamic Range performance. A selection of gratings and slits offers you the flexibility of configuring the instrument for a wide range of applications in the 200- 1160 nm range. From low light Fluorescence applications to demanding Raman applications, the AvaSpec-HERO is your ideal companion. With the high-speed USB3.0 and Gigabit Ethernet communication interface, the connection to your computer is fast and simple. The digital IO ports enabling external triggering, control of shutters, and pulsed light sources from the Avantes line of instruments are available as well.

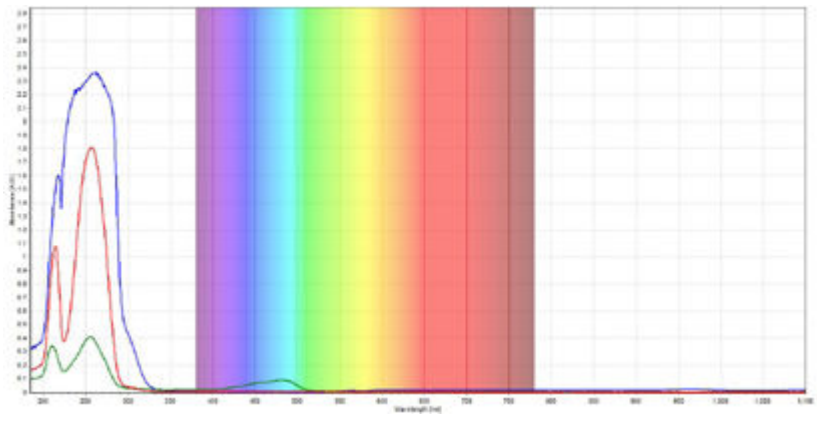
The AvaLight-DH-S is a powerful deuterium halogen source, but, like any unbalanced deuterium halogen source, it does have a very dominant alpha peak at 656 nm. Therefore, Avantes developed the DH-S-BAL, in which this peak is drastically reduced by a dichroic filter. This means less power, but an increase in the dynamic range of factor 20. The light source delivers a continuous spectrum with high efficiency. The highest stability is in the ultraviolet, visible, and near-infrared range, from 200 to 2500 nm. An integrated TTLshutter and filter holder for filters of up to 50 x 50 x 5.0 mm are included. The TTL-shutter can be controlled from any AvaSpec spectrometer, which means the auto-save-dark option in AvaSoft software can be used.

Methodology used:

For this experiment, we utilize the AvaSpec-HERO with an AvaLight-DH-S-BAL to measure samples in a 10mm pathlength cuvette. We test three different solutions of butylparaben in distilled water. The concentrations of the solutions are; 100ppm, 10ppm, and 1ppm. For our data collection, we will be utilizing the absorbance package in the AvaSoft software.

TEST DATA AND RESULTS

For this experiment, we utilize the AvaSpec-HERO with an AvaLight-DH-S-BAL to measure samples in a 10mm pathlength cuvette. We tested three different solutions of butylparaben in distilled water. The concentrations of the solutions are; 100ppm, 10ppm, and 1ppm. For our data collection, we utilize the absorbance package in the AvaSoft software.



Analysis:

Our setup utilized a long pathlength cuvette (10mm) to ensure the particles were visible. This proved to be an effective method, as the HERO was easily able to detect the butylparaben in each of the solutions. Cross-checking the data with that of known butylparaben absorbance spectra, the absorption peaks at 214 nm and 256 nm are exactly what is expected.

Conclusion:

The spectra from the three solutions prove that the AvaSpec-HERO is extremely suitable for collecting high-resolution spectra from samples and applications that require high sensitivity.

Curious to know more about particle detection in water? Contact us to see how we our solutions can help.

3.2.2 SPECTROSCOPY IN AGRICULTURAL & FOOD SCIENCES

Climate change and population expansion have a direct impact on agriculture. An increasing number of people need to be fed but changing weather patterns can cause complete crops to fail. Inevitably, farms must produce more with less, and frequently under increasingly difficult conditions. Growing seasons are shorter, there are fewer resources such as clean water, and even the soil itself can become depleted. Therefore, more and more players in the agricultural market turn to technology to help them work more efficiently and smarter, like spectroscopy. The last couple of years, we have seen an increase in applying this enabling technology in smart agriculture. Not only in research but also in agricultural equipment manufacturing, spectroscopy plays a key role. Because of the endless possibilities spectroscopy has to offer, it is applied in numerous applications that improve the future of agriculture. Below, we showcase a few applications in which spectroscopy enhances the outcome.

SOIL MANAGEMENT

Soil is a compound mixture of organic matter, minerals, gases, liquids, and even living organisms. In addition to supporting the plant life we need for crops, soil also functions as a means of storing, transporting, and purifying water; it helps to modify the atmosphere we all depend on and even serves as a habitat for organisms large and small. Sustainable soil management is as critical for future food production as it is for life on Earth.

Soil health is elemental to sustainable land management and is an important consideration for farms of all sizes. Anything from erosion to contamination, loss of biodiversity, soil compaction, and everything in between, can be detrimental to crop production and the viability of the farm itself. Numerous studies and technologies are in development for analyzing and managing soil health with the help of spectroscopy. Think about moisture measurement, soil characterization, and measuring bulk density and soil compaction.

FERTILIZER AUTOMATION

Not only for the plant but also for the soil the plant is on, it is important not to overapply fertilizer. Yara International ASA uses spectroscopy in a module that attaches to farm tractors used with their fertilizer applicators. They apply spectroscopic diffuse reflection, ideally suited to this application, as it requires limited hardware and performs at a very high speed (e.g., 600 spectra p.s.). The module measures the solar illumination and correlates this with reflection data from the crops. The reflected light from the crops provides rich information about the chlorophyll content, allowing for the derivation of a health score. This score regulates the fertilizer application level in real-time and also maps this to GPS coordinates for future monitoring. Yara's module provides an excellent example of spectroscopy's critical role in utilizing resources better and improving agricultural yields.

HEALTH MONITORING - DETECT DISEASES

NIR spectroscopy is proved a cost-effective and accurate method for detecting plant diseases at the leaf and canopy levels. For example, on the detection of Rice Blast Fungus. It is considered a significant threat to food safety and stability due to the severe yield loss that it causes. Until recently, the method for detecting rice blast was a physical inspection on the ground. It was time-consuming and nearly impossible for large-scale operations. With the help of NIR spectroscopy, correlation between rice blast disease index and IR spectra can lead to early detection technologies for large-scale operations. This allows for more efficient use of agrichemicals and a more sustainable method of crop management.

Researchers at the National Rice Research Institute and the Academy of Agricultural Sciences in China employed neural networks to analyze reflectance spectra in the development of their modelling for rice blast detection. Their aim was to detect spectral regions where rice reflectance changed, depending on rice neck blast disease index. But also to select the key wavelength bands and sensitivity to analyze disease severity and validated their neural network-based spectral model for qualifying disease severity[1].

QUALITY ASSESSMENT OF FRUIT

Researchers at the Polytechnic University of Valencia, use a spectrometer to develop a mango quality index for prediction modeling. They also use it to create a robotic gripper, capable of simultaneous tactile and NIR measurements to determine the quality and ripeness of the mango[2]. This non-destructive method of assessing fruit quality is based on the mango samples' biochemical and physical properties. Mangoes are typically not ready for consumption at the time of maturity. They require a period for ripening. During this period, many significant chemical and physical changes occur within the fruit. Diffuse reflectance spectroscopy was used with a fiber-optic probe in direct contact with the mango skin to measure the changes in soluble solids, ascorbic acid, water content, and color.

Spectroscopy has a place in every step of the food production cycle, from production to grading and sorting. By measuring plant health and acting accordingly based on the results, farmers can optimize their crop production.

FOOD OF THE FUTURE

Long-term space missions and Mars colonization projects will require producing food in less than optimal environments for plant growth. This has significant ramifications for planning to meet the dietary needs of these future colonies. The Laboratory of Environmental Biology and Life Support Technology, in partnership with the International Joint Research Center of Aerospace Biotechnology & Medical Engineering, is studying the effects of low-intensity light on the growth, photosynthesis, and yield of wheart[3].

The researchers used a spectrometer to control the light intensity of different test groups at the various growth stages. They discovered that low light at early growth stages had little effect on the ultimate yield so long as adequate light was available during the later grain filling stages.

References:

1. Zhang, Hao, et al. 'Estimation of rice neck blasts severity using spectral reflectance based on BP-neural network.' Acta physiologiae plantarum 33.6 (2011): 2461-2466.

2. Cortés, Victoria, Carlos Blanes, José Blasco, Coral Ortíz, Nuria Aleixos, Martín Mellado, Sergio Cubero, and Pau Talens. "Integration of Simultaneous Tactile Sensing and Visible and Near-infrared Reflectance Spectroscopy in a Robot Gripper for Mango Quality Assessment." Biosystems Engineering 162 (10 2017): 112-23. doi:10.1016/j.biosystemseng.2017.08.005.

3. Dong, Chen et al. 'Low light intensity effects on the growth, photosynthetic characteristics, antioxidant capacity, yield and quality of wheat (Triticum aestivum L.) at different growth stages in BLSS'. Advances in Space Research Volume 53, Issue 11, 1 June 2014, Pages 1557-1566

3.2.3 MORE APPLICATION NOTES

If you're interested in exploring more in-depth research and applications of spectroscopy in the environment, agricultural or food fields, we invite you to visit our website. There, you'll find a wide range of case studies and detailed insights into how spectroscopy is advancing innovations in detecting diseases, crop monitoring, air polution monitoring, and much more. Whether you're focused on environmental research, food applications, or agricultural sciences, our extensive library of application notes can provide valuable information to support your work. Explore more here.

3.3 Key Takeaways Environmental, Agriculture & Food

Spectroscopy has become a vital analytical tool in environmental, agricultural, and food sciences, offering rapid, non-invasive measurements that provide real-time data. Its ability to detect and quantify pollutants, assess soil health, and ensure food quality makes it indispensable in tackling today's global challenges, such as climate change and resource management.

From monitoring water contamination to improving crop yields, spectroscopic techniques like UV-Vis, NIR, and fluorescence spectroscopy deliver the accuracy and efficiency required for sustainable practices.

In environmental science, spectroscopy is essential for detecting pollutants in air, water, and soil, offering a detailed analysis of ecosystem health. Similarly, in agriculture, it aids in optimizing crop production, monitoring plant health, and improving soil management.

For the food industry, it ensures product quality and safety by detecting contaminants, assessing nutritional content, and verifying authenticity, enhancing the entire food supply chain.

Avantes' innovative solutions play a critical role in advancing these fields, offering flexible, high-performance instruments designed for a wide range of applications. To explore more case studies and spectroscopic applications in environmental, agricultural, and food sciences, we invite you to visit our website or contact our technical team for tailored advice.

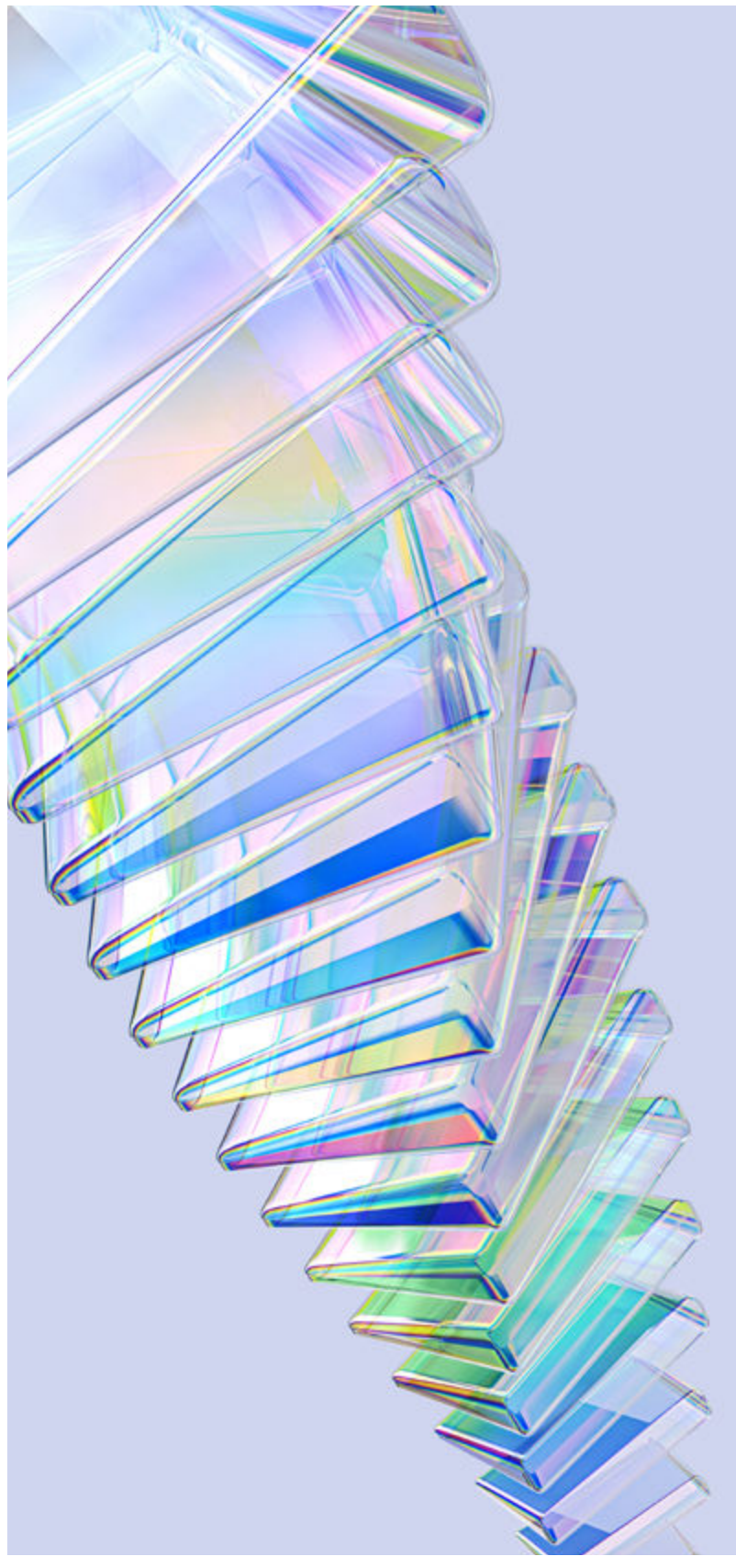
4

CHAPTER 4

MATERIAL SCIENCE

4.1 Introduction Spectroscopy in Material Science

Spectroscopy serves as an essential tool in materials science, providing deep insights into the composition, structure, and properties of various materials. Its non-destructive nature and high precision make it ideal for studying everything from polymers and metals to nanomaterials and semiconductors. By enabling real-time, in-situ analysis, spectroscopy facilitates the investigation of material properties under different conditions, such as temperature, pressure, and environmental stress. This allows researchers and manufacturers to optimize materials for specific applications and enhance the development of new, advanced materials.



In materials science, techniques such as Raman, and UV-Vis spectroscopy are frequently employed to analyze chemical bonds, molecular structures, and elemental compositions. Raman spectroscopy, for instance, is particularly valuable for characterizing carbon-based materials like graphene, while UV-Vis spectroscopy, on the other hand, plays a critical role in analyzing thin films, coatings, and nanoparticles. These spectroscopic methods provide essential data that inform the creation of stronger, lighter, and more efficient materials.

In this chapter, we will explore the various ways spectroscopy is applied in material science, showcasing a few real-world examples that highlight its impact on advancing technologies in various sectors.

4.2 Application Notes

4.2.1 SPECTROSCOPY IN MATERIAL SCIENCE

Spectroscopy can solve complex issues related to material degradation, corrosion, and failure, offering solutions for enhancing durability and extending the lifespan of materials. By providing real-time, in-situ data, spectroscopy accelerates the innovation process in material science, helping researchers develop stronger, more efficient materials for future technologies.

RAMAN VS. INFRARED SPECTROSCOPY FOR MATERIAL ANALYSIS (OCTASULFUR)

Infrared and Raman spectroscopy are both categorized as vibrational spectroscopies, which, broadly speaking, measure the same basic material properties. Namely, they provide a molecular fingerprint by determining the vibrational energy levels of a given material. The fingerprint is used to highlight the fact that for two materials to have the same vibrational spectra, they must have identical reduced mass, bond configuration, and steric effects. To put it more succinctly, the only way two samples can have the same vibrational spectra is for them to be the same material. Therefore, Raman and infrared spectroscopy are among the most used analytical techniques for unknown material identification and reaction monitoring.

Despite the surface-level similarities of the two techniques, in practice, there are many subtle (and not so subtle) differences, which have led many in the community to believe that one technique is superior to the other. This fracturing is rather unfortunate since the two techniques are highly complementary, and most laboratories can benefit from owning both Raman and infrared setups. To illustrate this, we have decided to focus this application note on determining which vibrational modes are better suited for Raman analysis and which ones are better suited for infrared.

A detailed analysis of the selection rules governing infrared and Raman spectroscopy can be somewhat overwhelming for those unfamiliar with quantum mechanics and physical chemistry. But most spectroscopists are familiar with the primary takeaways: infrared absorbance is a linear process dependent on the dipole moment, and Raman scattering is a nonlinear process dependent on polarizability. Armed with this basic understanding, we can utilize molecular symmetries to simplify the process. Although this requires knowledge of group theory, fortunately, only 32 different point (symmetry) groups are needed to characterize any possible molecular configuration, each having a well-defined character table that includes all possible translational, rotational, and vibrational operations for that group. Furthermore, the point group has already been identified and cataloged for most molecules.

HOW TO READ A CHARACTER TABLE

To illustrate the properties of a character table, we will use the relatively simple case of molecular octasulfur, the most commonly occurring sulfur in nature. Figure 1 shows octasulfur forms a crown-like ring of 8 atoms, each with equal bond lengths. From a simple visual inspection, it is apparent that this molecule is symmetric under several different possible transformations. For example, a rotation around the center of the ring by either 90^0 or 180^0 would leave the molecule completely unchanged. In group theory, these two symmetry operations are referred to as C_4 and C_2, where the general form Cn operation refers to rotation about the axis by $360^0/n$. While these two operations are the most obvious, they are not the only symmetries associated with octasulfur. For example, the molecule can be reflected through a dihedral plan (σd), it can be rotated by 450 and then reflected through the axis of symmetry (S_8), or it can simply not change at all (E).

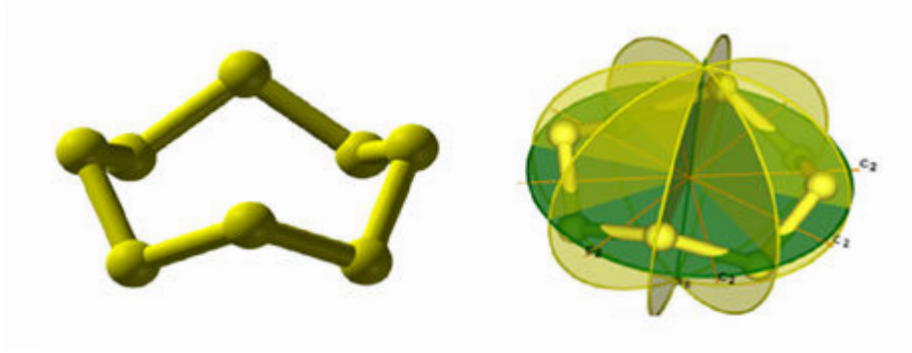


FIGURE 1 Chemical structure of octasulfur; with some of the symmetry operations in the D_{4d} point group

The 32-point groups, therefore, represent collections of all possible combinations of symmetry operations for a given geometry, and octasulfur falls into the D_{4d} point group. The details of the naming conventions for the point groups are not particularly important, but in this case, D_{4d} stands for a group containing a four-fold axis, four two-fold axes, and four dihedral mirror planes. Effectively this means that at least one C4 is allowable, four C_2', and four σdoperations, where the prime indicates rotation perpendicular to the primary axis. There are 16 possible symmetry operations for D_{4d} point group, known collectively as the group's order. While this may seem fairly complicated, character tables offer a simplified representation of all possible symmetry operations within the point group, which can be derived from the group multiplication table. Figure 2 shows the D_{4d} character table, which is broken up into two main parts, the first shows the various irreducible representations of the group and the second shows the basis coordinates of each representation.

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$		
A_1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	1	−1		
B_2	1	−1	1	−1	1	−1	1	z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	−2	0	0	(x, y)	
E_2	2	0	−2	0	2	0	0		(x^2-y^2, xy)
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	−2	0	0	(R_x, R_y)	(xz, yz)

FIGURE 2 D_{4d} character table

The letters in the first column of the character table, known as the Mulliken symbols for the irreducible representations, where A & B are symmetric and anti-symmetric with respect to the principal rotational axis. E, T, G, and H are used to denote two-, three-, four- and five-dimensional irreducible representations, but it should be noted that most point groups do not require dimensionality greater than two. It is also essential to pay close attention to whether E is used to denote the identity symmetry operation (top row) or the two-dimensional irreducible representation (first column).

While we will need to use all the information in the character table to eventually determine the allowed vibrational modes of our molecule, at this point, it is worth pointing out that a simple inspection of the basis coordinates can quickly determine if a mode can support infrared absorption or Raman scattering. Since, as stated previously, infrared is a linear process, only modes with a linear basis will be capable of supporting infrared absorption, which in our case corresponds to B_2 and E_1. By contrast, only A_1, E_2, and E_3 can support Raman scattering since they correspond to nonlinear basis coordinates. B_2, on the other hand, is known as a silent mode since it does not have a basis coordinate and therefore remains undetectable. While under certain circumstances, both Raman and infrared can be sensitive to rotational modes making A_2 potentially detectable, as with most introductory texts on this subject, we will ignore them since they do not correspond to molecular vibrations.

The last major takeaway that an initial inspection can make of this character table is that there are no infrared active symmetric modes or Raman active anti-symmetric modes. As it turns out, this trend is repeated across many point groups. While not a hard and fast rule, it is a reasonable first-order approximation to assume that symmetric vibrations are more Raman active and anti-symmetric vibrations are more infrared active.

DETERMINATION OF ACTIVE MODES

Before we can determine the total number of vibrational modes, we must first calculate the character of the reducible representations for our specific molecule of interest, which is done through inspection to identify how many atoms in the molecule are unaffected by each symmetry operation. Since octasulfur is a ring molecule with no center atom, all of our rotation operations (S_8, C_4, C_2, S_8^3, & C_2') will affect atoms, allowing us to set all of those terms equal to zero. We also know that, by definition, none of the atoms will be affected by the identity operation (E), so all eight will remain unaffected. The only tricky one to determine is the mirror operation (σd), but upon careful inspection, it can be determined to leave two atoms unaffected. Next, the character of each representation can be determined by multiplying the number of unaffected atoms by the total number of contributions per atom.

The trace of each transformation matrix determines the number of contributions per atom. This derivation is beyond the scope of this application note; however, the results are simple and easy to use. For the identity operation, the contributions per atom are always equal to 3, and for mirror operations, it is always equal to 1. To determine the number of contributions for a rotation operation (Cn) simply use the equation $1+2\cos(2\pi/n)$, and for an irregular rotation operation (Sn), use $2\cos(2\pi/n)-1$. While there are no inversion operations (i) as part of the D_{4d} point group, for the sake of completeness, we should note all inversion operations have a per atom contribution of -3. Therefore, we have a total reducible character of 24 for the identity operation, 2 for the mirror operation, and 0 for the rest (see table 1).

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$
Unaffected Atoms	8	0	0	0	0	0	2
Contribution Per Atom	3	$\sqrt{2}-1$	1	$\sqrt{2}-1$	-1	-1	1
Character of Reducible Representation (Γ_{red})	24	0	0	0	0	0	2

TABLE 1: Reducible Representation for Molecular Motion of Octasulfur.

$$\begin{pmatrix}\text{number of irreducible}\\ \text{representations of}\\ \text{a given type}\end{pmatrix} = \frac{1}{\text{order}}\sum\left[\begin{pmatrix}\text{number of}\\ \text{operations}\\ \text{in class}\end{pmatrix}\times\begin{pmatrix}\text{character}\\ \text{of reducible}\\ \text{representation}\end{pmatrix}\times\begin{pmatrix}\text{character of}\\ \text{irreducible}\\ \text{representation}\end{pmatrix}\right]$$

FIGURE 3: Irreducible representation equation

Using the equation shown in figure 3, we can determine the total number of irreducible representations for each type resulting in one representation of A_2 and B_1, two representations of A_1 and B_2, and three representations of E_1, E_2, and E_3.

Finally, to find the total number of vibrational modes, we must subtract out the translational (B_2 & E_1) and rotational (A_2 & E_3) representations, which can be determined using the basis vectors in the character table. As shown in Table 2, this leaves us with two A_1, one B_1, one B_2, two E_1, three E_2, and two E_3 vibrational modes. Since the E modes each represent two orthogonal modes with the same energy, these leave us with 18 total vibrational modes, which is consistent with the fact that nonlinear molecules contain 3N-6 vibrational degrees of freedom. These modes can then be further subdivided into five infrared active modes, one B_2 & two E_1, since they have a linear basis, twelve Raman active modes, two A_1, three E_2, & two E_3, which have a nonlinear basis, and one silent mode, B_1, which is lacking any basis.

Γ_{total}	2 A_1	A_2	B_1	2 B_2	3 E_1	3 E_2	3 E_3
$-\Gamma_{trans}$				B_2	E_1		
$-\Gamma_{rot}$		A_2					E_3
$=\Gamma_{vib}$	2 A_1		B_1	B_2	2 E_1	3 E_2	2 E_3

TABLE 2: Total number of vibrational modes

In vibrational spectroscopy, we are primarily interested in two types of vibrations– higher-frequency stretching and lower-frequency bending modes. The simplest way of differentiation between them is that stretching modes result from atoms moving back and forth along the bond axis. In contrast, bending modes result from deviations from the bond axis. Therefore, by transforming our coordinate system from a typical x-y-z cartesian system to a curvilinear coordinate system with motion restricted to the radial coordinate we can use group theory to identify the stretching modes. Since there will only be one degree of freedom this results in the contribution per atom from the identity operation reducing from 3 to 1. Using this new coordinate system, the reducible representation now becomes 8 for the identity operation, while remaining 2 for the mirror operation, and 0 for the rest. Following the same procedure as before, we now end up with eight stretching modes corresponding to A_1, B_2, E_1, E_2, and E_3. This means the ten remaining modes A_1, B_1, E_1, two E_2, and E_3 must all be bending modes.

$$\begin{pmatrix}\text{number of irreducible}\\ \text{representations of}\\ \text{a given type}\end{pmatrix} = \frac{1}{\text{order}}\sum\left[\begin{pmatrix}\text{number of}\\ \text{operations}\\ \text{in class}\end{pmatrix}\times\begin{pmatrix}\text{character}\\ \text{of reducible}\\ \text{representation}\end{pmatrix}\times\begin{pmatrix}\text{character of}\\ \text{irreducible}\\ \text{representation}\end{pmatrix}\right]$$

TABLE 3: Classification of vibrational modes

To experimentally demonstrate these results, we used an AvaSpec-HERO (also called AvaSpec-HSC1024x58TEC-EVO) configured to measure from 790nm to 1100nm with a 50µm slit and an AvaLaser785 ultra-high-throughput Raman probe with an integrated 785nm wavelength stabilized laser source (see figure 4). A two second integration was used without any signal averaging.

Based on the spectrum shown in figure 5, we are able to detect two distinct groupings of Raman bands. Based on our previous analysis, we can identify the lower-frequency cluster between 125cm-1 - 275cm-1 as the A_1, two E2, and E3 bending modes, and the higher frequency cluster between 400 cm-1 - 500cm-1 as the A1, E2, and E3 stretching modes. The peak visible below 100cm¬-1 is not a bending mode of the molecule, but a structural vibration resulting from octasulfur that forms an orthorhombic crystal at room temperature.

FIGURE 4: Set up of system with Raman 785 laser, AvaSpec-HSC, and sample holder

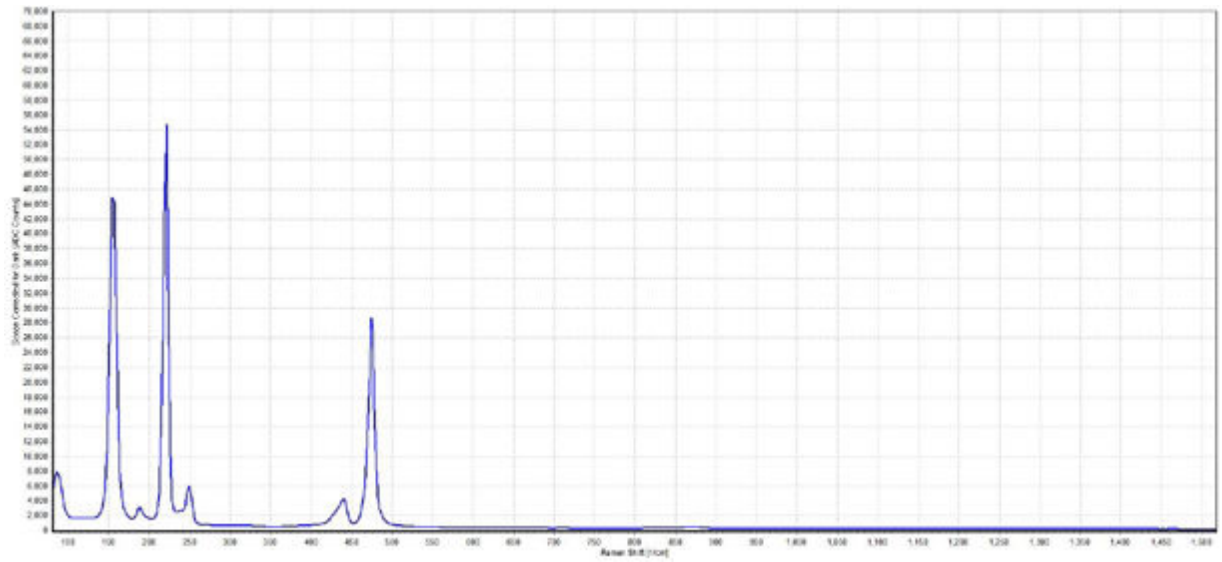


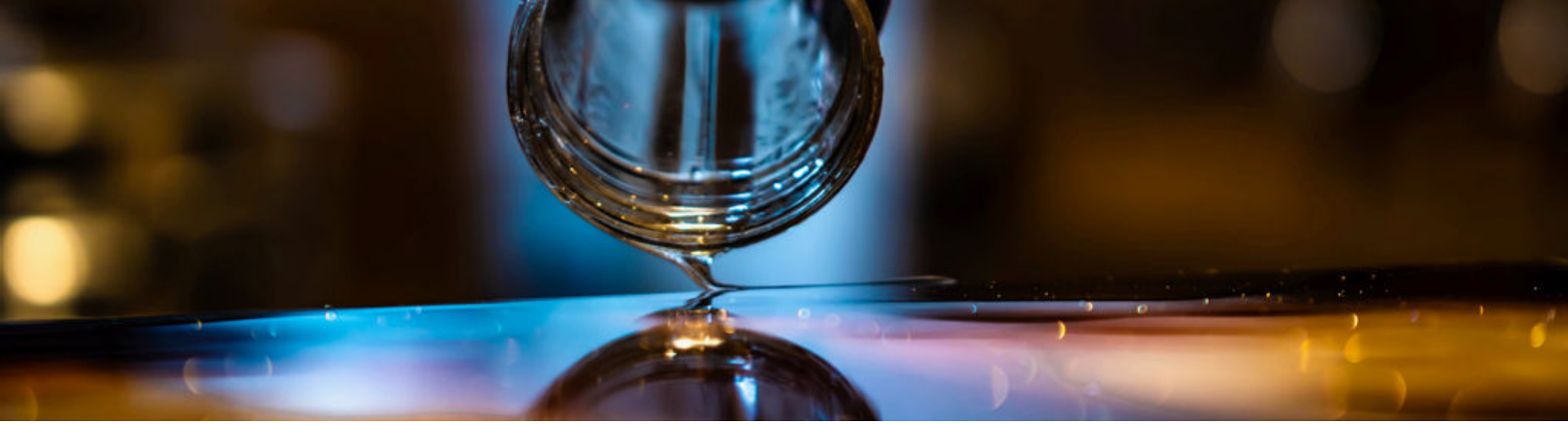
FIGURE 5: Raman spectrum of octasulfur

FINAL THOUGHTS

This analysis is intended to provide insight into how physicists and chemists can determine the vibrational modes of a given molecule based on its geometry and highlight the importance of using both Raman and infrared spectroscopy as complementary tools. We specifically chose to look at octasulfur to highlight the power of symmetry and group theory for determining the spectra characteristics.

Still, it is essential to remember that this approach can be applied to any molecule of interest. It is also important to note that while all the components used were standalone modules, they are also available as units OEM modules or can be integrated into multichannel rack mount systems. These units can communicate via USB, Ethernet, and the native digital & analog input/output capabilities of the Avantes AS5216 electronics board provides for a superior interface with other devices.

Additionally, the Avantes AS5216 DLL package, with sample programs in Delphi, Visual Basic, C#, C++, LabView, MatLab, and many other programming environments, enables users to develop their own code. For more information about our products, material analysis, and more, please contact us.



4.2.2 QUANTITATIVE ANALYSIS OF EPOXY RESIN WITH NIR

Discover the power of Near-Infrared (NIR) spectroscopy in understanding epoxy resin curing processes. Epoxy resins play a crucial role in industries ranging from manufacturing to 3D printing. Dive into this fascinating world with our application note. Learn how to monitor and quantify the curing of epoxy resin with NIR spectroscopy to ensure top-notch product quality and performance.

BACKGROUND INFORMATION

Epoxy resins have become so ubiquitous in modern society that the word epoxy has evolved into a generic term to describe industrial-strength adhesives. Unfortunately, this often leads to confusion since many industrial-strength adhesives are not epoxies, and not all epoxies are adhesives. Epoxy resins are widely used in various manufacturing applications since, when cured, they result in high-performance thermosets, highly crosslinked polymers. In addition, these resins are used as a background matrix in a wide range of composite materials and are finding increasing applicability in dual-cure additive manufacturing. For example, some of the newer high-performance 3D printer resins rely on interpenetrating polymer networks (IPNs) which are created by mixing photocurable (acrylate) resins with epoxy resins. Therefore, parts can be first "green printed" using vat polymerization or direct ink write methods and then thermally post-cured to kick off the epoxy polymerization process. While this incurs an extra processing step, IPN resins produce final parts with far superior thermal and mechanical properties when compared to traditional photo-cured resin systems.

Strictly speaking, epoxies are a broad class of molecules containing a triangular ring with one oxygen atom covalently bound to two carbon atoms. When combined with a molecule containing reactive functional groups, typically amines, it causes the ring to open and initiate the polymerization process. A prototypical two-step epoxy/amine reaction is shown in figure 1, whereby an epoxy monomer first reacts with a primary amine opening the ring and forming a secondary amine. Then the remaining secondary amine reacts with a second epoxy monomer creating a tertiary amine linking the two epoxy monomers together into a dimer. It should be noted that while this is somewhat of a simplification of the epoxy/amine polymerization process, ignoring effects such as etherification, it is more than sufficient for gaining an intuitive understanding of the process.

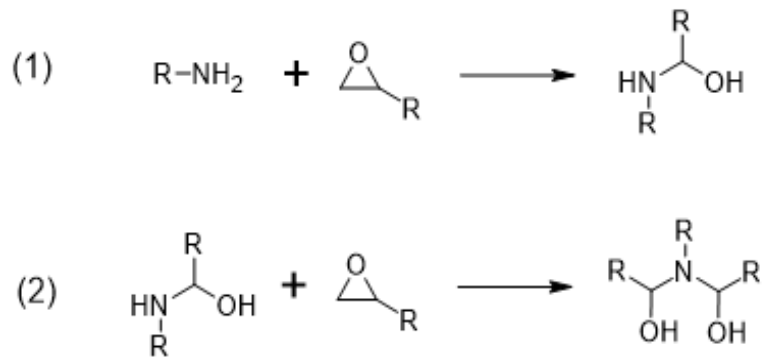


FIGURE 1: Chemical reactions between epoxy and amine monomers during resin curing, with (1) showing the primary amine reaction and (2) the secondary amine reaction.

MONITORING EXTENT OF CURE

Cure time is a critical parameter when it comes to epoxy processing. Whether it be a simple adhesive application or a high-performance composite, the cure kinetics ultimately govern the overall processing requirements during manufacturing. A wide variety of thermal/mechanical measurement tools have been employed for determining epoxy cure times, such as differential scanning calorimetry (DSC) and rheometry. But these approaches all suffer from a common downfall; not only are they destructive in nature they are also ill-suited for in situ applications and provide no direct information about the chemical reaction itself. For these reasons, vibrational spectroscopy has become the most common tool for measuring epoxy extent of cure. While it is possible to monitor epoxy polymerization using both Raman and mid-infrared (MIR) spectroscopies, neither of these methods are as analytically "clean" as near-infrared (NIR) spectroscopy. Since the three main functional groups of interest (epoxide, amine, & hydroxyl) are all highly polar, the Raman cross-section is extremely low. While the MIR absorption efficiency is relatively high, the presence of a broad peak at ~930 cm-1, which varies counter to the epoxy peak at ~915 cm-1, makes accurate quantitation nearly impossible without the use of deconvolution or other more advanced chemometric techniques. However, in the NIR spectral region, there is a clear separation between the epoxy peak at ~6100 cm-1, the amine peaks at ~6600 – ~6700 cm-1, and the hydroxyl peak at ~7025 cm-1. By normalizing the NIR absorbance spectra to the nearby CH band ~5900 – ~6000 cm-1, it's then very simple to track the three functional groups as they change during curing.

LAB-ON-A-CHIP SEPARATION CAPABILITIES

To demonstrate the effectiveness of using NIR spectroscopy to monitor the epoxy cure, we created an epoxy/amine resin prepared from a diglycidyl ether of bisphenol A resin, commercially known as EPON 828, and a diethylmethylbenzenediamine initiator, known as Epikure W. For easy handling and to ensure uniform thickness, and as a result, cure, sample wells were created on microscope slides using double-sided silicon tape, and the resin was pipetted into the well and then covered with a second microscope slide. The slides were then labeled 0, 1, 5, 10, 15, 30, 45, 60, 90, and 120 to indicate the time in minutes each sample would be cured at 180oC (see figure 2). An empty sample well was also created to serve as a reference. The experimental setup shown in figure 3 used an Avantes variable collimating lens holder mounted sideways to provide a sample platform for the absorption measurements. The AvaLight-HAL-S-Mini2 10W tungsten halogen lamp was coupled to a 200-micron core UV/IR broadband fiber-optic patch cord and connected to the lower collimating lens. The transmitted light was collected using the upper collimating lens, coupled into an identical fiber patch cord, and then measured using an AvaSpec-NIR512-1.7-HSC-EVO thermo-electrically cooled with a spectral range from 900 – 1700nm (11000 – 5880cm-1) with a 1.75ms integration time and no averaging.

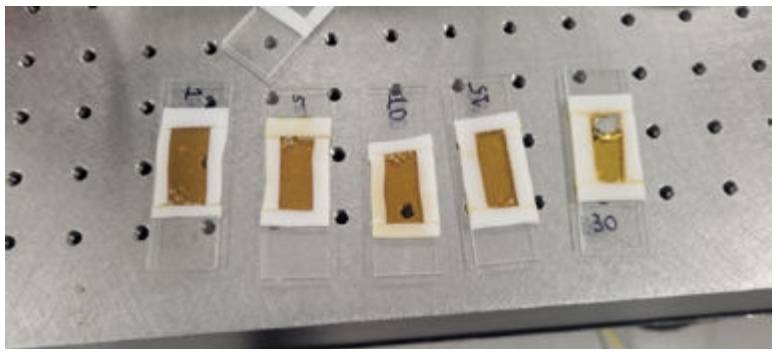


FIGURE 2: Example of sample preparation, showing 4 of the 10 epoxy samples prepared for this study

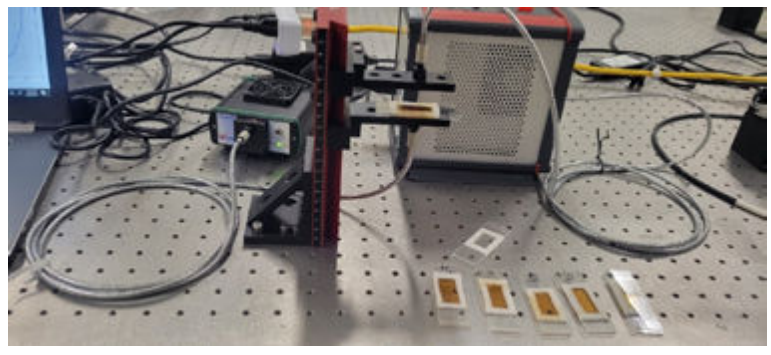


FIGURE 3: Experimental setup.

EXPERIMENTAL RESULTS AND DISSCUSSION

Figure 4 shows an overlay of the collected NIR spectra for varying cure times from 0 to 120 minutes. Initially, the spectrum contains a clearly visible epoxy ring peak at 6090 cm-1 and a primary amine peak at 6691 cm-1. Through the first 10 minutes of the curing process, both peaks steadily decrease without any noticeable appearance of secondary amine or hydroxyl bands. At the 15-minute mark, a clear shoulder begins to form at 6629 cm-1, correlating to a significant conversion of primary to secondary amines. At the same time, we have the first appearance of the hydroxyl band at 7016 cm-1. 30-minutes into the cure, the primary amines appear to have been fully converted to secondary amines. Throughout the remainder of the cure, the overall intensities of the epoxy ring and amine bands continually decrease, but the hydroxyl band tells a more complicated story.

As discussed in the previous section, while amine-induced ring opening is the primary driver of polymerization, etherification may also occur. The complex chemistry of epoxy/hydroxyl reactions is beyond the scope of this application note, but it is important to note that hydroxyl groups bound to tertiary amines can react with remaining epoxy rings to form quaternary ammonium polyether. Therefore, reducing the total number of hydroxyl groups, which can manifest as a reduction in the hydroxyl band. While this effect is difficult to confirm without more advanced spectral processing (due to baseline fluctuations), there does appear to be some fluctuation in the hydroxyl band intensity during the last hour of the cure.

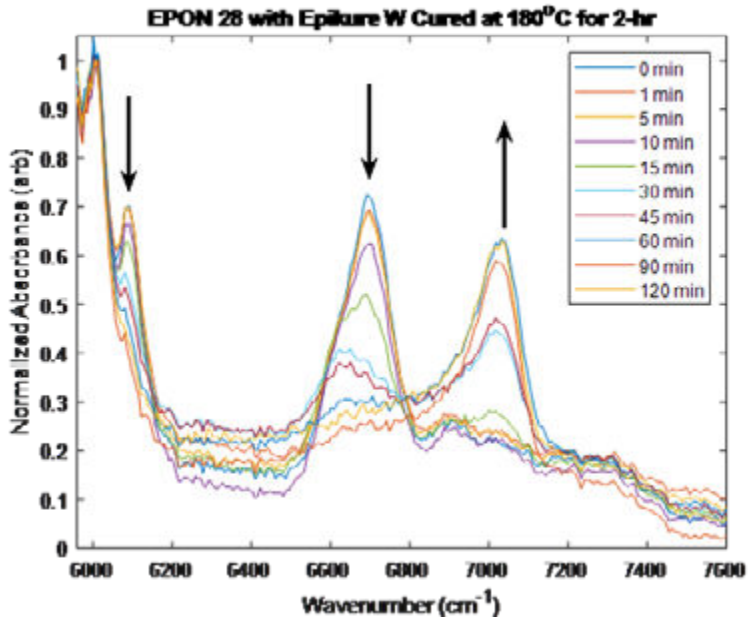


FIGURE 4: NNIR spectral overlay of 10 epoxy samples, with cure times varying from 0 to 120 minutes. All spectra are normalized to the CH band at 6007 cm^{-1}. No additional processing was used.

To demonstrate the quantitative capabilities of NIR spectroscopy to determine the extent of cure, we decided to calculate conversion α using the following relationship, $\alpha = 1 - \frac{I}{I_o}$ where *I* is the integrated intensity of the epoxy absorption band at 6090 cm^{-1}, and I_o is the integrated absorption of the unreacted sample (0 minutes).

In order to calculate the intensity, we utilized a simple 2-point linear baseline correction, as shown in figure 5 (left). The calculated conversion was then fitted to a simple phenomenological kinetic rate equation, $\frac{d\alpha}{dt} = k(\alpha_u - \alpha)^n$ using the MATLAB curve fitting toolbox (see figure 5 right). The ultimate conversion α_u was determined to be 1 (or 100%), the reaction order, n, was 1.1, and the rate constant, k, was 0.04.

It is important to note that, as discussed previously, epoxy/amine polymerization has extremely complex reaction kinetics; therefore, this simplistic rate equation is not necessarily an accurate depiction of the cure. However, since the purpose of this application note is merely to show the applicability of the methodology, it is more than sufficient for our purposes. The process could also be improved by increasing the sampling rate, using a more sophisticated baseline correction method, and accounting for the initial inhibition time (activation energy).

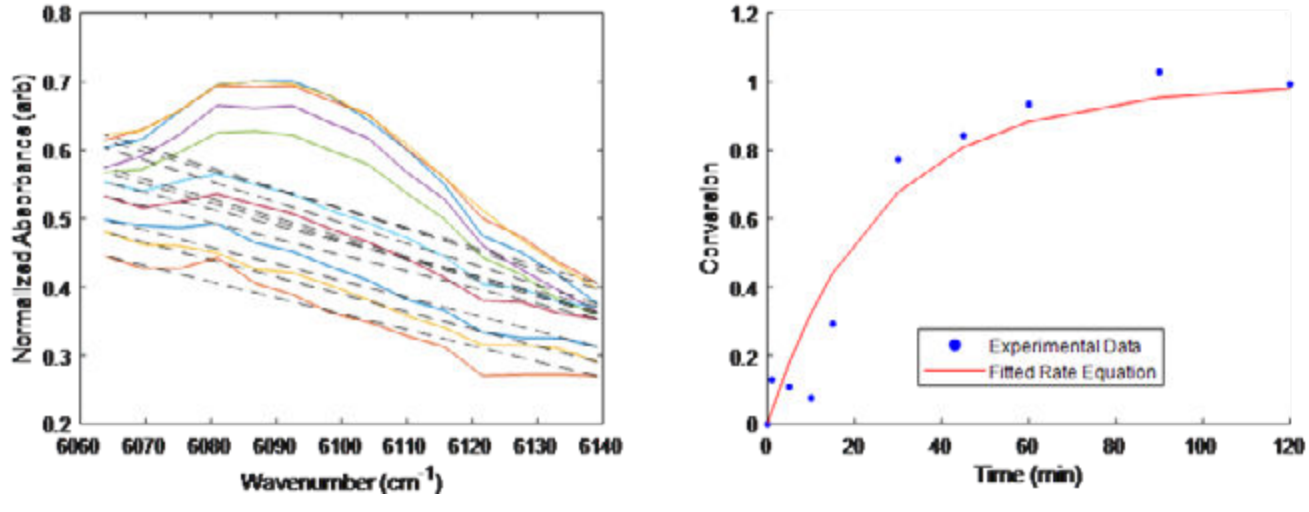


FIGURE 5: Zoomed-in view of the epoxy ring absorption band at 6090 cm^{-1} with the black dashed line showing the linear baseline fit. All spectra are color-coded in accordance with the previous figure. (left) Epoxy cure conversion in blue, fitted to a phenomenological kinetics rate equation in red. (right) I.[2]

FINAL THOUGHTS

An accurate understanding of cure kinetics is essential for developing a holistic understanding of the structure-property-processing relationships of epoxy resins. While several analytical methods can be used to monitor the extent of cure and determine the relevant kinetic constants, NIR spectroscopy is by far the simplest and most accurate. While in this study, we only utilized a 1.7-micron InGaAs-based sensor; it is important to note that Avantes offers spectrometers capable of measuring up to 2.5 microns. By expanding the spectral range to 2.5 microns, users can measure NIR absorption spectra down to 4000 cm-1, providing access to a standalone primary amine band at ~4930 cm-1 and an additional epoxy band at ~4530 cm-1. While, as we have demonstrated, neither of these bands is required for measuring the epoxy extent of cure, they can be helpful since the ~4530 cm-1 absorption band is far stronger and better resolved than the 6090 cm-1 band. Additionally, the ~4930 cm-1 standalone amine band can be rather useful if you are interested in gaining a deeper insight into the conversion of primary to secondary amines.

4.2.3 MORE APPLICATION NOTES

If you're interested in exploring more in-depth research and applications of spectroscopy in material science, we invite you to visit our website. There, you'll find a wide range of case studies and detailed insights into how spectroscopy is advancing innovations in quality control, and material analysis. Our extensive library of application notes can provide valuable information to support your work. Explore more here.

4.3 Key Takeaways Material Sciences

Spectroscopy has evolved into a vital tool for materials science, offering detailed insight into chemical composition, molecular structure, and dynamic reactions in a variety of materials. This chapter has highlighted how spectroscopy provides a multi-dimensional view of material properties and transformations, utilizing a spectrum of methods—Near-Infrared (NIR), Raman, and Infrared (IR) spectroscopy among others—to cater to specific analytical needs.

Through studies on epoxy resin curing and sulfur analysis, we saw how NIR and Raman spectroscopy complement each other in identifying complex reactions and composition-specific insights. NIR's ability to monitor real-time changes in resin curing and the strengths of Raman for inorganic analysis underscore spectroscopy's flexibility across different applications.

As spectroscopy technologies advance, especially in integration and data processing, the field promises even greater insight into materials, encouraging innovative approaches to real-time monitoring and analysis in research and industry.

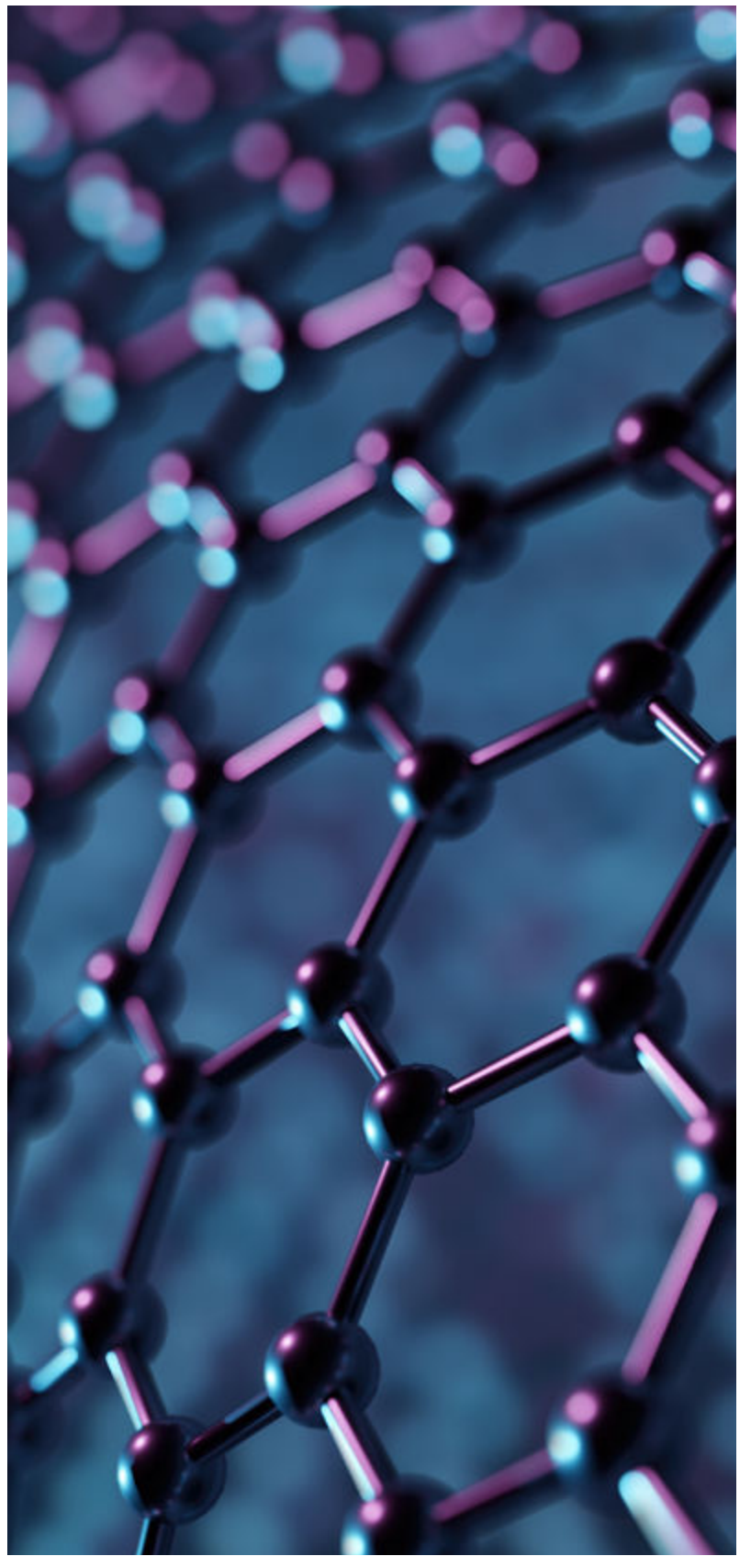
Need help finding the right solution for your application? Our team is here to guide you through the world of spectroscopy, so you can select the best techniques and tools for your unique material analysis needs.

Visit our website to discover our product portfolio, or contact our technical engineers for advice. We are happy to help you!

5

CHAPTER 5
CHEMISTRY & NANOTECHNOLOGY

5.1 Introduction Spectroscopy in Chemistry & Nanotechnology



In chemistry and nanotechnology, spectroscopy offers unparalleled insights into molecular interactions, reaction dynamics, and nanoscale structures. By enabling detailed analyses at atomic and molecular levels, it aids researchers in understanding reaction mechanisms, chemical bonding, and the properties of nanomaterials with high precision. Techniques like Infrared (IR) and Raman spectroscopy shed light on vibrational and rotational energy levels, essential for identifying chemical composition and structural properties in nanomaterials and complex compounds.

In chemistry, spectroscopy supports the investigation of reaction kinetics, catalysis, and molecular synthesis, driving innovations in areas ranging from pharmaceuticals to renewable energy. In nanotechnology, these techniques help characterize nanoparticles, and thin films, critical for developing materials with tailored electronic, optical, and mechanical properties. Raman, for instance, is a go-to method for analyzing carbon-based nanostructures, while UV-Vis spectroscopy is instrumental in studying the optical characteristics of quantum dots and other nanomaterials.

This chapter dives into the two applications of spectroscopy in both chemistry and nanotechnology, such as carbon quantum dots, highlighting how it contribute to the synthesis, characterization, and functional optimization of materials. Through practical examples, we'll explore how spectroscopic data guides advancements in these dynamic fields.

5.2 Application Notes

5.2.1 CHEMICAL IDENTIFICATION WITH RAMAN SPECTROSCOPY

Raman spectroscopy is a highly valuable and widely utilized technique for real time chemical identification measurement in various molecules and materials. Its non-destructive, rapid, and precise results have made it indispensable across diverse industries such as Pharmaceutics, Forensics, Food, Chemistry and Materials science, Gemstone identification, and Petrochemical identification.

It is important to emphasize that proper calibration methods are being applied for chemical identification measurements to ensure accurate and reliable identification and data interpretation. Therefore, distinct calibration models are required to ensure accurate wavelength, Raman shift and intensity. Once a reliable calibration is performed, it becomes feasible to obtain chemical information based on the peak position, intensity, shift, and width. By leveraging the Avantes Raman spectrometer, an efficient, non-destructive, and accurate chemical detection system can be achieved.

As an example, it is shown here that Raman spectroscopy can be used to identify the chemical structure of specific resins used in the industry. Specifically, the detection of aromatic bonds within the structure are highlighted. Depending on the case, the recommended setup includes the Avaspec-HSC1024x58TEC-EVO, either having a larger wavelength range, or having a better resolution but with a reduced wavelength range.

INTRODUCTION

Raman spectroscopy is a powerful technique for studying the chemical structure and properties of material and molecules. It is based on the elastic, and the inelastic scattering of photons by molecules. When a laser is directed at a sample, for example a resin, the molecules scatter the light. Most of this scattered light has the same frequency (elastic scattering) as the incident laser light, a phenomenon known as Rayleigh scattering. However, a minor yet crucial fraction of the light is inelastically scattered, undergoing a change in frequency. This change is known as Raman scattering.

The principle of Raman spectroscopy lies in detecting these frequency shifts in the scattered light. These shifts occur due to the transfer of energy between the photons and the vibrational energy levels of the molecules in the sample. When molecules vibrate, they modify the energy of the scattered photons, resulting in either a decrease (Stokes) or increase (anti-Stokes) in energy. This energy shift directly correlates with the vibrational frequencies of the molecules.

The resulting Raman spectrum contains specific peaks and shifts that reveal various molecular properties, including:

1. **Peak position:** Known as the Raman shift is measured in wavenumbers (cm-1) and corresponds to the vibrational and rotational modes of the molecules.

2. **Intensity:** The height of the peak provides information on the amount of substance (e.g. concentration, film thickness, crystalline/amorphous ratio, etc).
3. **Peak shift:** Shifting of the peak compared to a reference position can provide information on the mechanical stress within the material.
4. **Line width:** The width of the peak provides information on the quality of the material (e.g. crystallinity, impurities, defects).
5. **Polarization:** When polarized light is used, information can be obtained on the symmetry and orientation within the material.

Chemical identification using Raman spectroscopy is being used in many industrial applications:

1. **Pharmaceutical Analysis:** In the pharmaceutical industry, Raman is extensively used for the identification and verification of drug substances and formulations. It can quickly identify active pharmaceutical ingredients (APIs), detect polymorphic forms, and assess the quality and authenticity of pharmaceutical products.
2. **Forensic Science:** In forensic investigations, Raman is employed to identify unknown substances found at crime scenes, such as drugs, explosives, and trace evidence. It helps law enforcement agencies and forensic scientists quickly determine the chemical composition of evidence.
3. **Food and Beverage Quality Control:** Raman is used in the food and beverage industry for quality control and safety assessment. It can detect contaminants, analyze nutritional content, and verify the authenticity of food products.
4. **Environmental Monitoring:** In environmental monitoring and pollution analysis, Raman plays a vital role. It can identify pollutants, assess soil and water quality, and monitor air pollution by detecting specific compounds.
5. **Art and Archaeology:** Raman is utilized in art restoration and archaeology to identify pigments, binders, and other materials used in artworks and artifacts. This helps in preserving and conserving cultural heritage.
6. **Material Science:** In material science research, Raman is used to study the structure and composition of various materials, such as polymers, nanomaterials, ceramics, and crystals. It provides insights into molecular bonding and structural properties.
7. **Gemstone Identification**: Raman is employed in gemology to distinguish between natural and synthetic gemstones and to identify different types of gem materials based on their chemical composition.
8. **Medical Diagnostics:** Raman has potential applications in medical diagnostics, including the identification of disease biomarkers, characterization of tissues, and early detection of diseases.
9. **Petrochemical Analysis:** In the petroleum and petrochemical industry, Raman is used for identifying hydrocarbons, analyzing crude oils, and assessing the quality of fuels.

To perform chemical identification using Raman spectroscopy, some important steps are typically followed. The spectrometer needs an accurate Wavelength Calibration which can be performed using specific calibration light sources. (e.g. Argon, Krypton, or Xenon). Such calibration ensures the light falling onto a specific pixel of the detector correspond to the correct wavelength number. Although the wavelength of the laser is specified, there is always a slight deviation which can lead to a small shift of the Raman spectra and thus to falls data interpretation. Therefore, calibrating the full system and the Laser wavelength is needed, which can be done by measuring material with a clear distinct Raman spectrum. Such reference sample could include Sulphur, Polystyrene, Cyclohexane, or Polytetrafluoroethylene (PTFE).

For certain applications also an Intensity calibration of the detector is required in order to obtain the correct ratio between peak areas. This could be obtained by measuring and referencing a white light spectrum, or by performing an Irradiance calibration.

EXAMPLE ON RESINS

Resins play a critical role in industries such as paints, varnishes, inks, coatings and adhesives. How well they perform within their application depends on their chemical structure. Resins are organic compounds composed mainly of polymers formed by interconnected monomeric units. They find widespread use in coatings, adhesives, and plastics due to their excellent adhesive properties. Resins can be natural or synthetic, with natural resins derived from plant sources and synthetic resins manufactured from petrochemicals. Additionally, there are aliphatic and aromatic resins. Aliphatic resins are characterized by their straight or branched chain hydrocarbon structures, while aromatic resins contain one or more benzene rings within their molecular structure.

Raman spectroscopy provides insights into the molecular structure of resins. It reveals information about chemical bonds, functional groups, and molecular configurations, which are essential for understanding resin properties related to adhesion, strength, and flexibility. In a mixture, the compatibility between resins and the other components is crucial. Raman spectroscopy helps assess the compatibility by analyzing interactions and molecular-level changes in the Raman spectra. As resins are classified as either aliphatic or aromatic, it is important to be able to distinguish between them within a Raman spectra as this information assists in choosing resins that exhibit optimal properties and/or compatibility in the final product. To highlight the feasibility of Raman spectroscopy to chemically identify resins, different types were analyzed using different spectrometer setups.

MATERIALS & METHODS

Spectrometer 1:

Specification	Description
AvaSpec	HSC1024X58TEC-EVO
AvaBench	USB3 - EVO-RS - 100mm
Grating	SI - 830 lines/mm
Detector	S7031-1024x58
Range (nm)	786,49 - 1020,04
Raman shift (cm\\\\-1)	32-2896

Spectrometer 2:

Specification	Description
AvaSpec	HSC1024X58TEC-EVO
AvaBench	USB3 - EVO-RS - 100mm
Grating	NB - 600 lines/mm
Detector	S7031-1024x58
Range (nm)	785,68 - 1132,57
Raman shift (cm\\\\-1)	32 - 3889

Light source:

Light source type	Light source name
785 nm	IPS laser

Samples:

Hydrocarbon Resin	Aromaticity
1	No
2	Yes
3	Yes
4	Yes
5	Yes

TABLE 1: List of Hydrocarbon resins measured using Raman spectroscopy

Polyterpene Resins	Aromaticity
1	No
2	No
3	No

TABLE 2: List of Polyterpene resins measured using Raman spectroscopy

Method:

Parameter	Value
Slit (µm)	25
Integration time (ms)	5000
Averaging	1
Smoothing	0

RESULTS

Below the spectra of the different Resins are presented, showing the results for Hydrocarbon Resins in Figure 1, and the Polyterpene Resins in Figure 2.

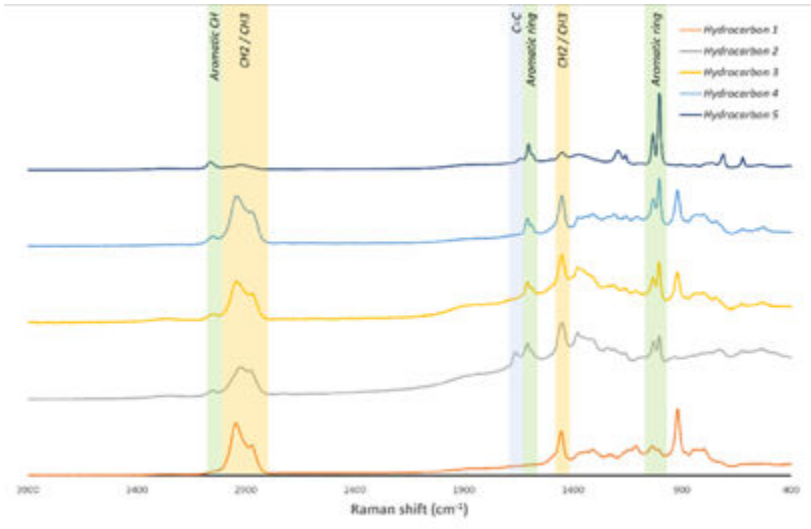


FIGURE 1: spectra of Hydrocarbon resins as measured using spectrometer setup 2. Specific regions of interest are highlighted and indicated to which part of the chemical structure it belongs.

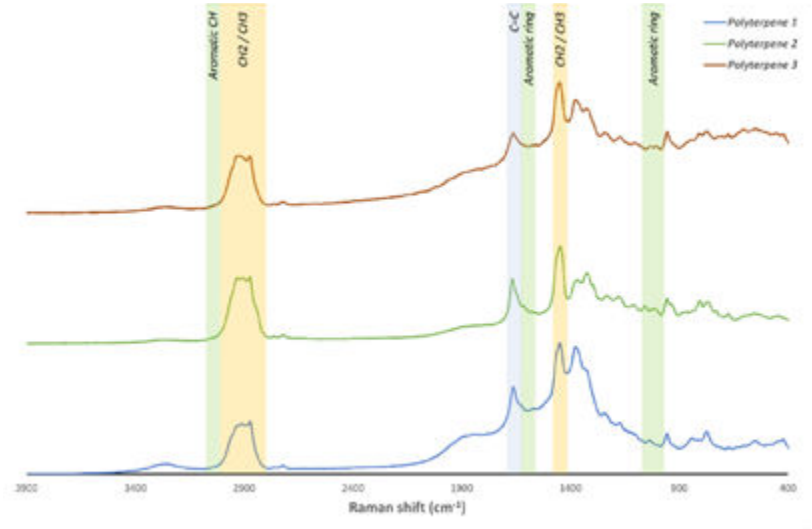


FIGURE 2: Raman spectra of Polyterpene resins as measured using Spectrometer setup 2. Specific regions of interest are highlighted and indicated to which part of the chemical structure it belongs.

The spectra displayed in Figure 1 reveal that the Hydrocarbon resins share comparable characteristic peaks. Similar can be said about the Polyterpene resins in Figure 2. Nevertheless, each resin possesses its own distinctive peaks, which can be attributed to its unique chemical structure or specific functional groups present.

Hydrocarbon resin nr 1 for example does not possess the distinct aromatic peaks, indicating that this resin is a fully aliphatic resin (Figure 2). On the other hand, Hydrocarbon nr 5 possesses a significantly higher ratio between the peaks from the aromatic bonds and the aliphatic bonds, compared to the other hydrocarbon resins. This indicates that Hydrocarbon resin nr 5 has the highest aromaticity than the other resins.

Within the Polyterpene resins one can see slight differences within the aliphatic regions. Indicting that there could be different ratio between the amount of methyl (-CH3) and methylene (-CH2-) groups. Additionally, one can see if the resin is saturated or unsaturated by looking at the peak around 1660 cm\\-1. A higher peak indicates a more unsaturated structure.

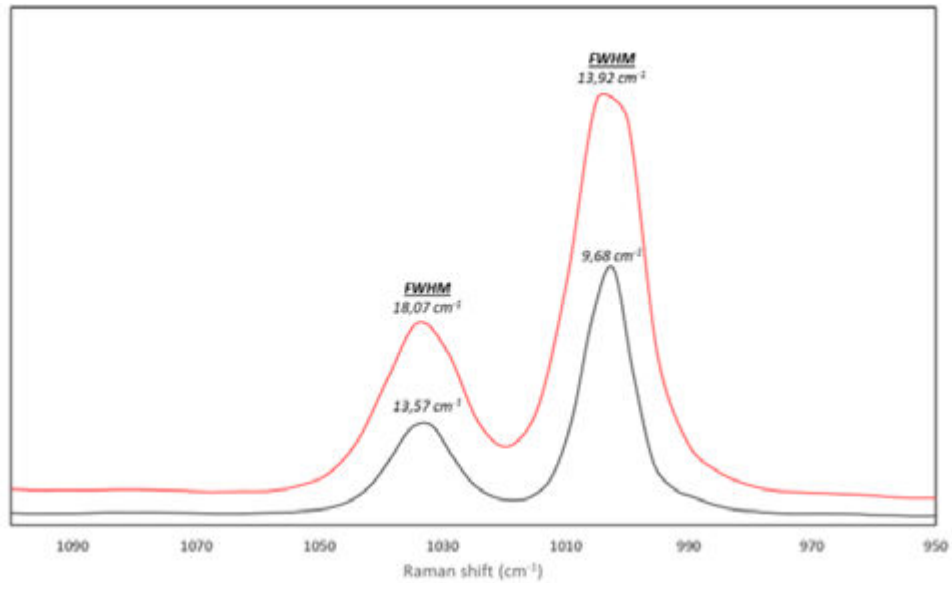


FIGURE 3: Spectra of Hydrocarbon 5, zoomed in at the peaks around 1020 cm-1, measured with 2 different range spectrometers to compare the resolution. Black line is spectrometer 1, and Red line is spectrometer 2.

To compare the spectra recorded with the two different Raman systems, and look at the resolution, the full width half maximum (FWHM) was measured (Figure 3). For this, the two strong Raman peaks at 1000 cm-1 and 1030 cm-1 were investigated (Table).

Full width half max	1000 cm^{-1}	1030 cm^{-1}
Spectrometer 1	9.68	13.57
Spectrometer 2	13.92	18.07

The investigated FWHM shows that depending on the range of the spectrometer as well as the starting wavelength it is possible to record either the full spectral range from 400 cm-1 till 4000 cm-1, or record a smaller range with a higher resolution.

CONCLUSION

Resins that are widely used in the industry can be easily measured using an Avantes Raman system.

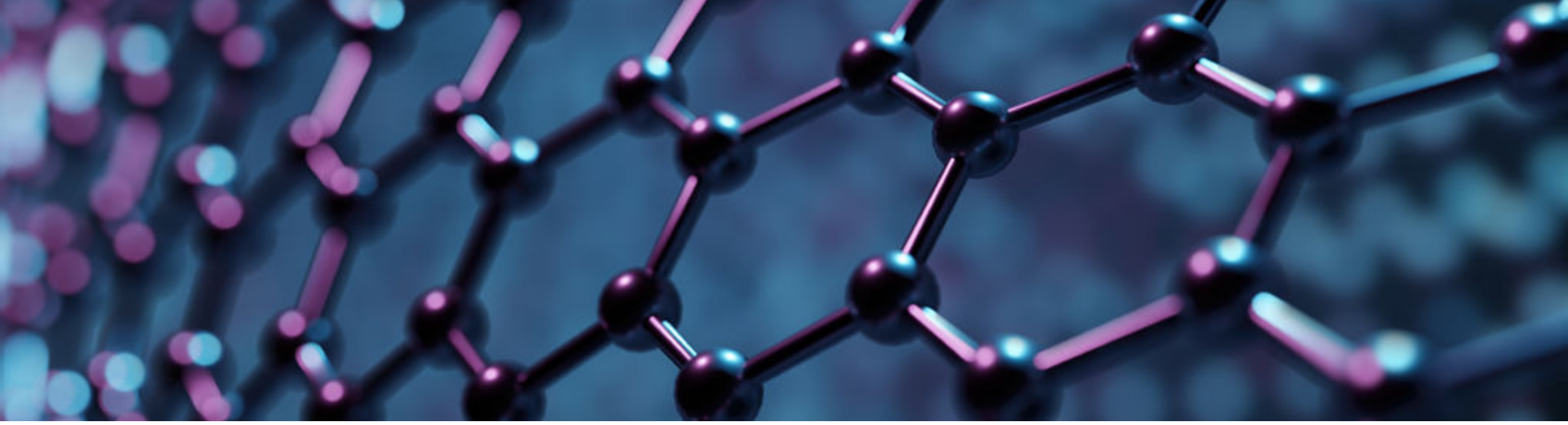
The spectra were first measured using an Avaspec-HSC1024x58TEC-EVO which had a detector with a shorter wavelength range, and therefore a shorter Raman shift range. This setup was able to measure from around 30 till 2900 cm\\-1. Clear peak separations were visible and significantly different spectra were recorded for the various resins.

Additionally, the same resins were recorded with another Avaspec-HSC1024x58TEC-EVO which had a large wavelength range, and therefore could measure up to a larger Raman shift. This setup was able to measure from around 30 till 3900 cm\\-1. For this system also significantly different spectra were recorded for the various resins.

When a proper peak assigning is performed, it will be possible to distinguish between the amount of aliphatic and aromatic carbon-carbon bonds. Additionally, one can investigate the variation in unsaturation between the various resins. All this information together would give the researcher the possibility to understand and predict the interaction and compatibility between the resin and the other components in a final product.

To compare the spectra recorded with the two different Raman systems, and look at the resolution, the full width half maximum (FWHM) was measured. For this, the two strong Raman peaks at 1000 cm\\-1 and 1030 cm\\-1 were investigated. It showed that by sacrificing on the range, a better resolution can be obtained.

Depending on the final application or requirements, Avantes can provide Raman systems that can easily distinguish between the different resins and provide information on the chemical structure of such components.



5.2.2 ADVANCES IN CARBON QUANTUM DOTS: SYNTHESIS, APPLICATIONS, AND SPECTRAL ANALYSIS WITH AVANTES

Over the past four decades, quantum dots have evolved from a scientific curiosity into a cornerstone of modern nanotechnology, finding applications across a wide array of fields, including biotechnology, electronics, and energy. Among these, carbon quantum dots (CQDs) have garnered significant attention due to their unique properties, such as tunable fluorescence, biocompatibility, and environmentally friendly synthesis. Unlike traditional semiconductor quantum dots, which often pose toxicity concerns, carbon quantum dots offer a safer alternative, opening new possibilities in biomedical imaging, drug delivery, and sustainable energy solutions.

As research in this area progresses, the ability to precisely characterize and control the optical properties of carbon quantum dots has become increasingly important. This is where spectroscopy plays a crucial role. Through advanced spectroscopic techniques, researchers can gain deeper insights into the emission profiles, structural properties, and chemical compositions of carbon quantum dots. These insights not only facilitate the development of new applications but also ensure the consistency and scalability required for commercial adoption.

This application note explores the latest advancements in carbon quantum dots, from their synthesis and surface engineering to their wide-ranging applications in nanotechnology and energy. We will also delve into the critical role of spectroscopy in understanding and optimizing these materials, demonstrating how Avantes spectrometers can support researchers and manufacturers in harnessing the full potential of carbon quantum dots.

INTRODUCTION

Traditional quantum dots are simply individual semiconductor nanocrystals where quantum confinement effects can be utilized to tune their fluorescence emission profiles. In the case of bulk semiconductors (i.e., LEDs and laser diodes), the minimum energy required to excite an electron to the conduction band and, subsequently, energy released through electron-hole recombination is dictated by material composition. However, when an electron-hole pair, referred to jointly as an exciton, is confined within a space commensurate with the de Broglie wavelength, which is typically on the order of 10 nm at room temperature. It behaves as a "particle in a box." This process, known as quantum confinement, causes the bandgap energy and therefore, the emission wavelength to change as a function of particle size. Building off the energy levels of a particle in an infinite square well potential (aka particle in a box) $E_n = \frac{h^2 n^2}{8mL^2}$ where n is the energy level, h is Plank's constant, m is the particle's mass, and L is the width of the well. The emission wavelength λ can be determined using,

$$\lambda = \frac{hc}{E_{g,bulk} + \frac{h^2}{8r^2}\left(\frac{1}{m_e^*} - \frac{1}{m_h^*}\right)}.$$

In Equation 1 ***c*** represents the speed of light, $E_{g,bulk}$ the band gap energy of the bulk semiconductor, ***r*** is the radius of the quantum dot, m_e^* the effective mass of the electron and m_h^* is the effective mass of the hole.

Based on this relationship, as the size of the dot decreases, so too does the emission wavelength, providing an exceptionally high degree of control over the emission wavelength, as shown schematically in Figure 1. It should also be noted that m_e^* and m_h^* are not the actual masses of the particles (holes have no mass); instead, they are related to the curvature of the energy-momentum relationship, which plays the equivalent role of the mass of a particle in a box. However, these values are extremely well characterized and can simply be looked up for a particular material. For example, in CdSe nanocrystals that m_e^* and m_h^* are 0.13 and 0.45 times the mass of an electron, and 0.07 and 0.50 times the mass of an electron, respectively in bulk GaAs.

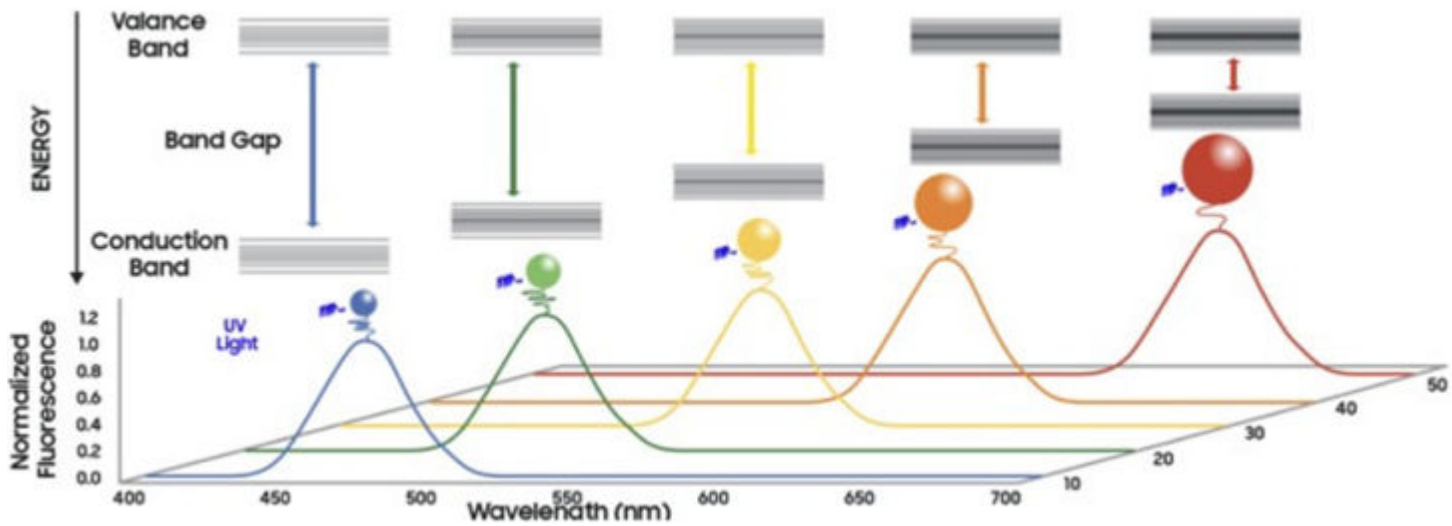


FIGURE 1: Schematic Illustration of the relationship between quantum dot, size, bandgap and emission spectra.

THE RISE OF QUANTUM DOTS

The high tunability, quantum yield, and narrow linewidth make quantum dots highly desirable as fluorescent tags, particularly for in vivo diagnostics. However, it is undesirable to inject II-VI semiconductors such as CdSe into human patients due to the potential toxicity. Fortunately, in 2004 Xiaoyou Xu and others at the University of South Carolina produced "Fluorescent Single-Walled Carbon Nanotube Fragments," which we now understand to be carbon quantum dots[1]. Driven mainly by a combined desire for biocompatibility and greener synthesis techniques over the last 20 years, there has been an explosion in carbon dot research. In fact, it has recently been shown that carbon dots can be synthesized from nearly any organic material ranging from orange juice[2] to upcycled polypropylene[3]. There is even recent evidence showing that carbon dots are produced (and inhaled) from electronic cigarettes[4].

CARBON DOTS SYNTESIS AND APPLICATIONS

Carbon dots are produced through hydrothermal treatment of any carbon-containing material. While this is typically done in an autoclave, it can also be done through laser ablation of carbon in solution. Researchers at the Universities of Messina and Enna have recently created carbon dots by focusing a 350mJ pulsed 970nm laser with a 10Hz repetition rate into a solution of charcoal dissolved in phosphate-buffered saline (PBS)[5]. Using an Avantes AvaSpec-2048-USB2 spectrometer (now available as AvaSpec-VARIUS) and a 365nm UV emission lamp they were able to demonstrate blue fluorescence with a spectral peak at 478 nm, as shown in figure 2.

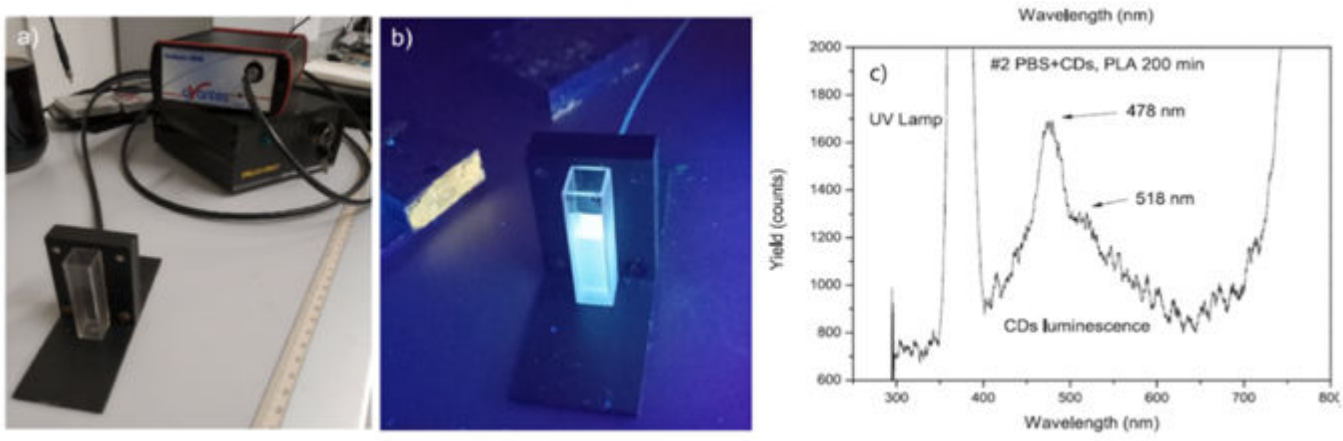


FIGURE 2: Experimental set-up luminescent under UV illumination (b), and emission spectrum when excited at 365 nm(c).[5]

These impurities can further complicate the HOMO-LUMO structure, leading to greater absorption and emission wavelength inexactness. However, this feature can also be utilized judiciously to tune the emission wavelength. For example, in a study published this summer (2024), a collaboration between the University of Munich, Trieste, and Leiden yielded blue-emitting boron- and nitrogen-doped carbon dots.[7] By incorporating these dots into thin-films, they were able to produce extremely bright white light emitting electrochemical cells with quantum yields of 42%. To verify the coatings' photostability and conversion efficiency, the electro-luminescence spectra were measured using an Avaspec-2048-USB2 coupled with an AvaSphere 30-Irrad Integrated sphere.

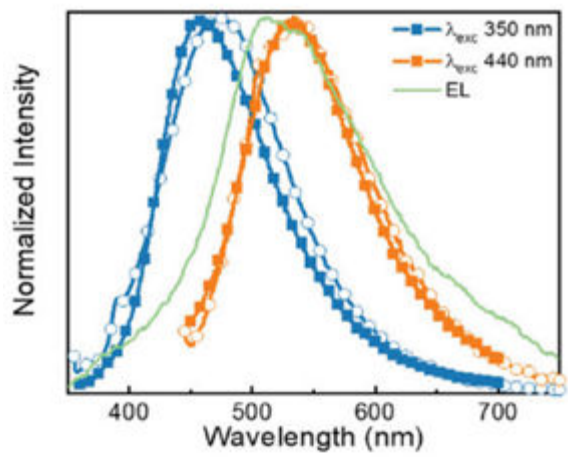


FIGURE 3: Normalized emission intensity of boron- and nitrogen-doped carbon dots excited at of 350 nm (blue) and 440 nm (orange) and the electro luminescence spectrum (green).[7]

Another particularly interesting use case was the recent collaboration between the Universities of Palermo and Messina in Italy, which demonstrated the ability to use microporous poly(D,L-lactide) acid–carbon nanodot (PLA-CD) nanocomposite scaffolds for image-guided bone regeneration.[6] In this work, they were able to quantify the amount of carbon dots successfully incorporated into the scaffolding by using an Avantes AvaSpec-VARIUS with a dual halogen-deuterium light source to monitor absorbance at 450nm and comparing it to a calibration curve produced by dissolving the dots in dichloromethane.

FUTURE APPLICATIONS USING CARBON DOTS

Carbon quantum dots are poised to transform a wide variety of scientific applications. For example, their biocompatibility, low toxicity, and eco-friendliness make them particularly appealing for biomedical applications, including bioimaging and drug delivery. Carbon dots are currently being used in several clinical trials mainly in oncology, where photoactive drugs are functionalized with carbon dots, enabling the targeted delivery of photodynamic therapies. They have also been demonstrated as a means of gene delivery and treating neurological disorders.

Furthermore, the recent advancements in the synthesis of carbon dots provide precise control over their emission spectra, opening doors to their use in light-emitting diodes (LEDs) and photovoltaics. The ability to fine-tune their emission spectra through doping and surface engineering has further expanded their utility in creating more efficient solar cells and white light-emitting diodes. They also can be used in energy storage by enhancing specific capacitance, energy density, and durability. Early work in osmotic power generation even hints at a future where carbon dots could play a pivotal role in sustainable energy solutions.

THE RISE OF QUANTUM DOTS

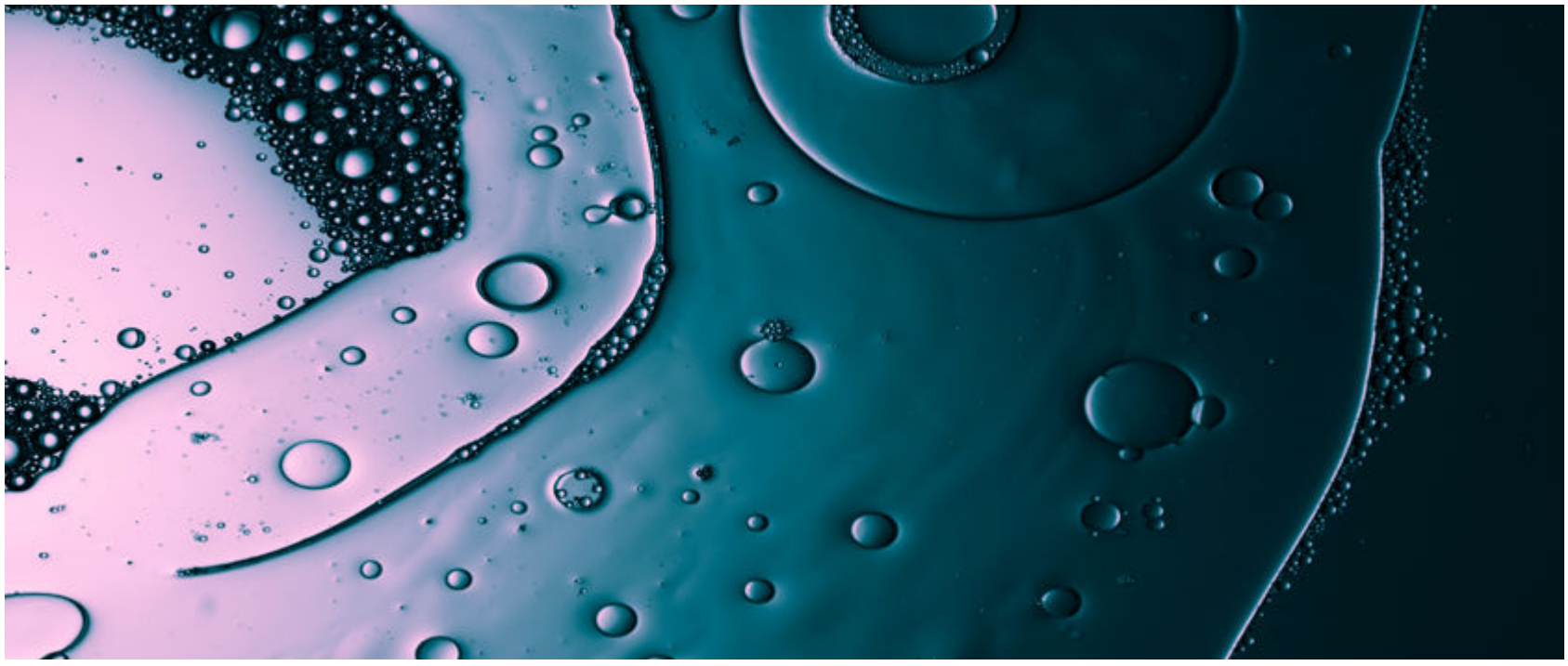
While commercial applications of carbon dots are still in the nascent phase, ongoing research is focused on overcoming challenges such as scalability and integration into existing technologies. As these hurdles are addressed, carbon dots will lead to breakthroughs in sensors, electronics, and environmental applications, marking them as a cornerstone in the future of nanotechnology. Avantes spectrometers are ideally suited to help facilitate these developments, particularly as production volumes increase, requiring large-scale batch analysis of absorption and emission spectra.

REFERENCES

1 J. Am. Chem. Soc. 2004, 126, 40, 12736–12737 https://doi.org/10.1021/ja040082h
2 Chem. Commun., 2012,48, 8835-8837 https://doi.org/10.1039/C2CC33796G
3 ACS Materials Lett. 2024, 6, 1968−1976 ttps://doi.org/10.1021/acsmaterialslett.3c01419
4 Biophysical journal. , 2024, Vol.123(3), p.437a https://doi.org/10.1016/j.bpj.2023.11.2653
5 Optics and Laser Technology 177 (2024) 111089 https://doi.org/10.1016/j.optlastec.2024.111089
6 Materials 2024, 17(2), 449; https://doi.org/10.3390/ma17020449
7 Adv. Optical Mater. 2024, 2400618 DOI: 10.1002/adom.202400618

5.2.3 MORE APPLICATION NOTES

If you're interested in exploring more in-depth research and applications of spectroscopy in chemistry & nanotechnology, we invite you to visit our website. There, you'll find a wide range of case studies and detailed insights into how spectroscopy is advancing innovations these areas. Our extensive library of application notes can provide valuable information to support your work. Explore more here.



5.3 Key Takeaways Chemistry & Nanotechnology

Spectroscopy has become essential in chemistry and nanotechnology, offering an intricate view of molecular structures, chemical interactions, and nanoscale properties. This chapter has underscored how spectroscopy serves as a bridge between chemistry and technology, revealing critical insights into the atomic and molecular world.

From Raman-based resin analysis to the spectral study of carbon quantum dots (CQDs), we've seen how spectroscopy provides clarity on complex reactions and nanostructures. Raman spectroscopy's ability to identify molecular characteristics in resins supports precise chemical development, while spectral analysis in CQD research highlights how nanoscale properties can be tailored for diverse applications—from bioimaging to renewable energy.

As spectroscopic techniques continue to advance, their potential to drive discoveries in chemistry and nanotechnology grows, supporting everything from fundamental research to industry applications.

Need guidance on optimizing spectroscopy for your applications? Explore our portfolio or connect with our experts today!

6

CHAPTER 6
FUTURE OF SPECTROSCOPY IN RESEARCH

The future of spectroscopy in research looks increasingly promising as technological advancements push the boundaries of what these techniques can achieve. As researchers continue to explore new frontiers in fields like materials science, environmental monitoring, biomedical diagnostics, and even space exploration, spectroscopy will play a pivotal role in driving innovation.

In the near future, we can expect advancements in spectroscopy to facilitate breakthroughs in personalized medicine, where real-time molecular analysis could help tailor treatments to individual patients.

Moreover, the development of quantum-based spectroscopic techniques promises to enhance the sensitivity and accuracy of measurements at the atomic and sub-atomic levels, allowing researchers to study matter with unprecedented detail.

As spectroscopy continues to evolve, it will remain a critical tool across many scientific disciplines, enabling researchers to address global challenges, from sustainability and climate change to energy efficiency and healthcare. Its ability to offer non-invasive, real-time, and highly sensitive measurements ensures its relevance in the decades to come.

Discover what implementing spectroscopy can do for your application by contacting one of our technical support engineers. We are happy to help you innovate in your area of expertise! Contact us here.

7

CHAPTER 7

AVANTES SOLUTIONS & DEMO PROGRAM

Avantes offers a versatile range of high-performance spectroscopy products tailored to meet the unique demands of industries from biomedical research to materials science and environmental monitoring. Our product portfolio includes a variety of spectrometers, light sources, fiber-optic accessories, and software, each designed to deliver precision, reliability, and adaptability for a wide array of applications. In this chapter we showcase a selection of our portfolio, to give you an insight into our solutions. If you like to see our whole portfolio, we advice you to visit our website.

To help you find the best fit for your needs, Avantes also provides a **demo program** that allows you to test select instruments directly within your lab or production environment. This program offers the flexibility to explore our technology firsthand, ensuring you have the right tools to achieve accurate, high-quality results in your work. Read along to discover more about our demo program.

7.1 CompactLine Spectrometers

Spectroscopy redefined, that is what we consider our CompactLine spectrometers to be. In applications where size matters, the CompactLine offers spectrometers with one of the smallest form factors on the market, such as the NEXOS™. The CompactLine enables easy integration into OEM and handheld devices.

The powerful and lightweight NEXOS™ spectrometers provide top-notch performance for spectroscopy integration, with high signal-to-noise ratio.

Equipped with CMOS detectors and advanced electronics and communications, these spectrometers offer both high resolution and speed. Multiple in multiple variations.

BENEFITS

- Customizable performance
- Easy to integrate
- Suited for harsh environments
- Compact size
- Temperature and wavelength stability
- 2048 or 4096 pixel detector
- High unit-to-unit reproducibility
- Superior stray light performance

7.2 StarLine Spectrometers

The StarLine family of high-performance Avantes spectrometers exceeds the needs of most general spectroscopy applications in the UV and visible ranges. This line includes high-speed instruments suitable for use in process control, high-resolution instruments for optical emission spectroscopy, and versatile solutions for irradiance and absorption spectroscopy, and other common applications.

The StarLine instruments are fully integrated with our modular platform, allowing them to function as both standalone and multi-channel instruments. The entire StarLine is available as an individual lab instrument, as well as an OEM module for integration into customers' existing systems.

BENEFITS

- Superior straylight rejection
- Fast integration time
- High resolution
- USB powered
- High-speed communication
- 2048 or 4096 pixel detector
- Improved sensitivity
- Ideal for general applications

7.3 SensLine Spectrometers

The SensLine includes ultra-high resolution, low-noise instruments ready for customers needing higher performance for demanding applications with back-thinned and TE-cooled options. The back-thinned CCD detectors featured in this line are high-quantum efficiency detectors with excellent response in the ultraviolet, visible, and near-infrared range from 200 to 1160 nm. The SensLine is designed for demanding applications like fluorescence, luminescence, and Raman.

All SensLine instruments are fully integrated with our modular platform, allowing them to function as both standalone and multi-channel instruments. Every instrument in this product line is available as a lab instrument or an OEM module

BENEFITS

- Superior straylight rejection
- High stability
- Low noise
- Thermo-electrically cooled
- High sensitivity
- Temperature stability
- Widest dynamic range
- High speed acquisition

7.4 NIRLine Spectrometers

Instruments in our AvaSpec NIRLine are high-performance, near-infrared spectrometers that are optimized for the demands of measuring long wavelengths. This line provides leading-edge performance for dispersive NIR instruments with toroidal focusing mirrors and dynamic dark correction for enhanced stability.

Options include uncooled, back-thinned CCD detectors out to 1700 nm or InGaAs detectors with thermo-electrical cooling suitable for measurements to 2500 nm. Instruments in the NIRLine are available as lab instruments or OEM modules for integration into customers' existing systems.

BENEFITS

- Superior straylight rejection
- High stability
- Low noise
- Thermo-electrically cooled
- High sensitivity
- Temperature stability
- Widest dynamic range
- High speed acquisition

7.5 Product Portfolio

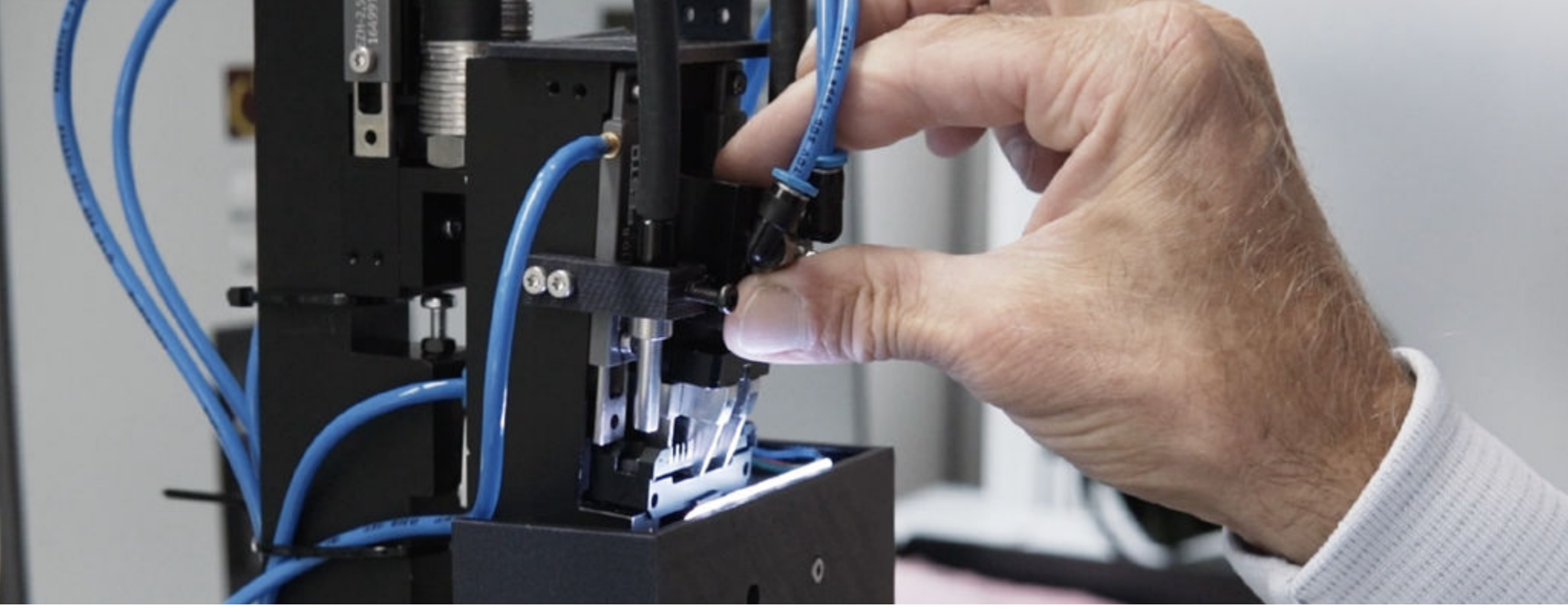
Beside spectrometers, we offer a wide range of products to complete your measurement setup.

Light Sources
Avantes' light source options include deuterium, tungsten halogen, and LED for spectral ranges from 190 nm – 2500 nm. The AvaLight line consists of several calibration sources for irradiance and spectral line calibrations. All light sources are fiber optic coupled with SMA connectors. More information? Click here.

Fiber Optics
We offer an extensive line of fiber optic cables, bundles, and probes. Our in-house production facility manufactures fiber optics for deep UV, UV/VIS, and VIS/NIR applications using high-quality silica fibers. Custom configurations for fiberoptic reflection, absorption, and fluorescence probes are always negotiable. More information? Click here.

Software
AvaSoft software is a 32 and 64-bit compatible application-oriented software package that enables complete control over our spectrometers. Application-specific software solutions are available. Our in-house engineers can work with customers to support standard and custom application needs (DLL). More information? Click here.

Accessories
We offer a wide range of fiber optic coupled sampling accessories such as cuvette holders, integrating spheres, filters, filter holders, and flow cells. In addition, Avantes offers a variety of fiber optic accessories, including collimating lenses, cosine correctors, and vacuum feedthroughs. More information? Click here.



AVAMATION: FUTURE-PROOF MANUFACTURING

There is a worldwide increasing demand for spectrometers. More and more customers purchase in large volumes, which means that the performance of each spectrometer must be exactly the same. Historically our spectrometers are assembled by hand with great precision and expertise, but with AvaMation, we semi-automated our manufacturing process. We decided to innovate this process to increase our efficiency and precision so we are ready for a future with an increasing demand of spectrometers.

This new way of manufacturing not only benefits Avantes when it comes to efficiency, but also yields the following benefits for its customers.

WHAT'S IN IT FOR YOU?

Scalable manufacturing capabilities
From small, up to very high volume orders, with AvaMation we are very flexible when it comes to customizing orders.

Superior inter-instrument reproducibility
Through AvaMation we not only take quality assurance to a higher level, but also provide more manufacturing precision and speed.

Enabling data analysis
By collecting data from the manufacturing process, we can continue to innovate and make product improvements in the future.

More information
Do you want to know more about AvaMation? Click **here** to read all about it.

7.5 Our Demo Program

TRY BEFORE YOU BUY

We understand the importance of getting it right when making an instrument purchase decision. Sometimes applications have special needs that are not known in advance. Our demo program allows you to test an spectrometer, light source, and even some accessories in your experiment or operation to validate functionality and fine-tune specifications. Vetting our instruments in your applications ensures you will be successful after you make a purchase. In the rare event, we don't meet or exceed your measurement demands, we eliminate the need for costly returns and reworks.

COMPARE WITH AN EXISTING INSTRUMENT

Often our customers have experienced a competitive or different class of instrument and would like to have a comparison to see if their measurements can be improved or cost-optimized. Demanding applications such as fluorescence and Raman are often performed with high-cost instrumentation which may be overkill for the needs of the applications. Our instruments raise the bar of performance such that our more affordable technology can replace higher cost, slower systems.

FINE TUNE SOFTWARE INTEGRATION & CONTROL

Our demo program allows you to familiarize with our software or take a closer look at our software development kit (SDK) and sample programs. Our instruments can be controlled using our proprietary software AvaSoft or via your own software written in Labview, Matlab, C#, C++, Visual Studio, Python, or any of a variety of Linux environments.

MORE INFORMATION

Interested in trying out our products? Contact one of our technical support engineers to make a reservation. Click here to fill out the form on our website.

SUPPORT & ADVICE

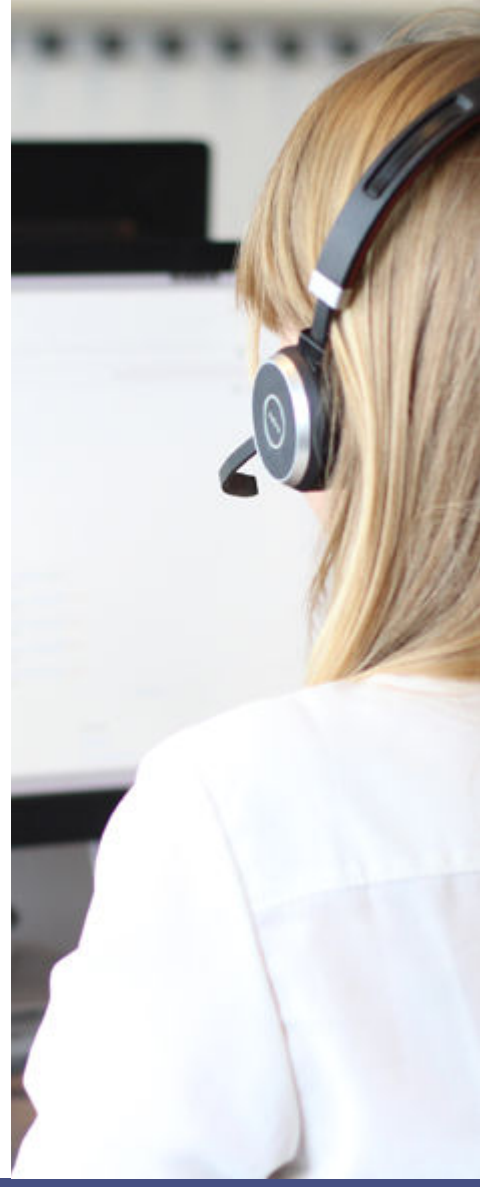
Providing high-quality equipment is only part of what we do. The other equally important factor is the high level of service we deliver. Our organization includes various specializations to provide you with the best service and advice:

Feasibility studies
Our sales engineers perform free feasibility studies to find your most ideal measurement setup.

Support team
Our support team never sleeps and provides you with the best possible service.

MyAvantes
A platform where you'll find AvaSoft Software and other helpful material for you to download.

Online support
Helpful documents and tutorial videos for extra help with your products.



DISCOVER MORE EBOOKS

Avantes makes an impact with spectroscopy technology all over the world. You can encounter our technology in the agricultural sector, the medical sector, and also in the solar energy and semiconductor market. Every market demands a different approach. But in every market, we contribute to science and enable our partners to make huge strides in quality, efficiency, and research.

We conducted four eBooks containing application examples, experiments and product information to showcase the endless possibilities spectroscopy offers in these markets.

Scan the QR-codes below to download our free eBooks.

Chemistry

(Bio)Medical

Environmental

Agriculture

AVANTES
MEMBER OF THE NYNOMIC GROUP

CONTACT

WE'RE HAPPY TO HELP

Curious how spectroscopy can help you reveal answers by measuring all kind of materials, in-line, at your production facility, in a lab or even in the field? Please visit our website or contact one of our technical experts, we're happy to help you.

Avantes Headquarters
Phone: +31 (0) 313 670170
Email: info@avantes.com
Website: www.avantes.com

Avantes USA office
Phone: +1 (303) 410 8668
Email: infoUSA@avantes.com
Website: www.avantesUSA.com

Avantes China office
Phone: +86 10 845 740 45
Email: info@avantes.com.cn
Website: www.avantes.cn

Follow us on social media: