



APPLICATION NOTE

CHEMICAL IDENTIFICATION WITH RAMAN SPECTROSCOPY (RESINS)



INTRO

SUMMARY

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 Pharmaceuticals, 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:** Raman spectroscopy is extensively used in the pharmaceutical industry 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:** Raman spectroscopy is employed in forensic investigations 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 spectroscopy 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:** Raman spectroscopy plays a vital role in environmental monitoring and pollution analysis. It can identify pollutants, assess soil and water quality, and monitor air pollution by detecting specific compounds.
5. **Art and Archaeology:** Raman spectroscopy 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.

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6. **Material Science:** In material science research, Raman spectroscopy 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 spectroscopy 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 spectroscopy has potential applications in medical diagnostics, including the identification of disease biomarkers, characterization of tissues, and early detection of diseases.
 9. **Petrochemical Analysis:** Raman spectroscopy is used in the petroleum and petrochemical industry 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.

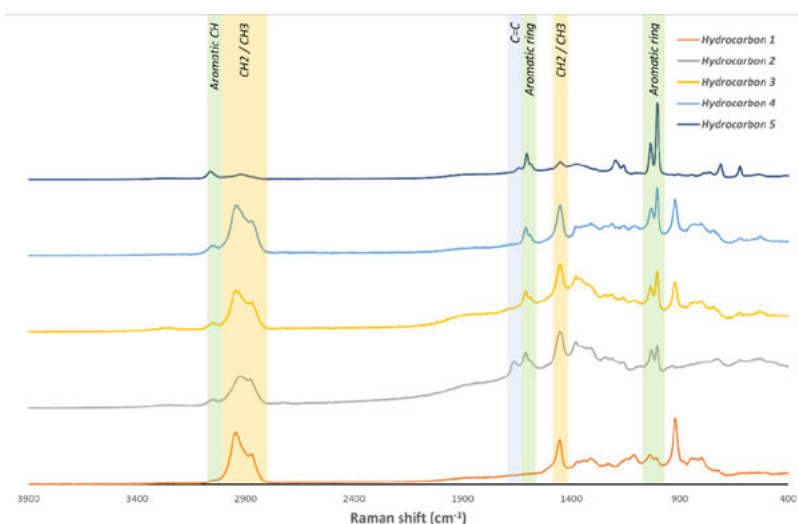


FIGURE 1: Raman spectra of Hydrocarbon resins as measured using Spectrometer setup 2. Specific regions of interest are highlighted and indicated to which part of the chemical structure it belongs.

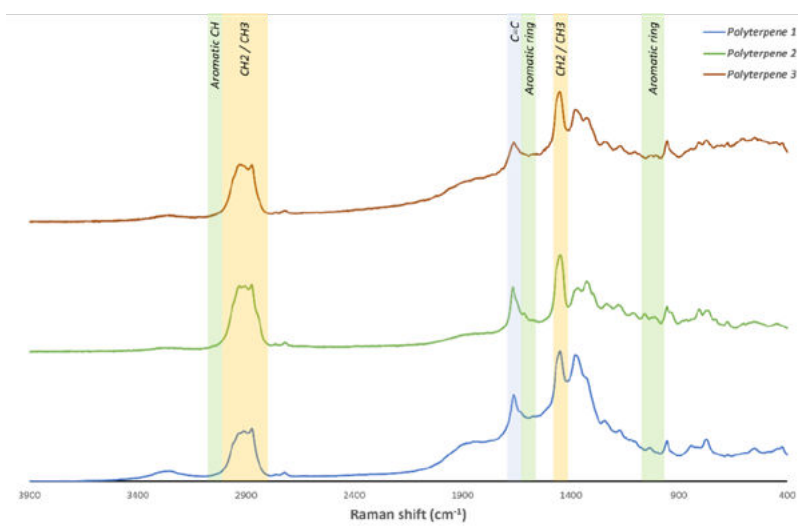


FIGURE 2: Raman spectra of Polyterpene resins as measured using Spectrometer setup 2. Specific regions of interest are highlighted and indicated to which part of the chemical structure it belongs.

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. Indicating 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.

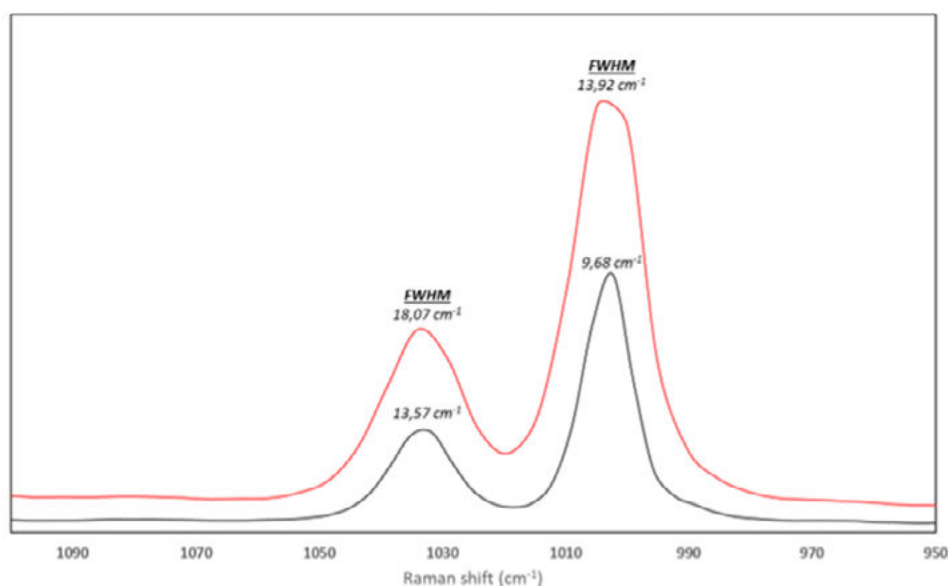


FIGURE 3: Spectra of Hydrocarbon 5, zoomed in at the peaks around 1020 cm⁻¹, measured with 2 different range spectrometers to compare the resolution. Black line is spectrometer 1, and Red line is spectrometer 2.

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.

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