RAMAN SPECTROSCOPY
APPLICATIONS

Easy-to-use and cost effective analytical method

Raman spectroscopy is a well-known method for chemical analysis and investigation of physical properties. This method was discovered in 1928 by Indian scientist Sir Chandrasekhara Raman and was named in his honor. Raman spectroscopy is used in a number of different techniques and useful applications.

Below is a short list of use cases for Coda Devices' Raman portable spectrometers.

RAMAN SPECTROSCOPY APPLICATIONS

Use Cases

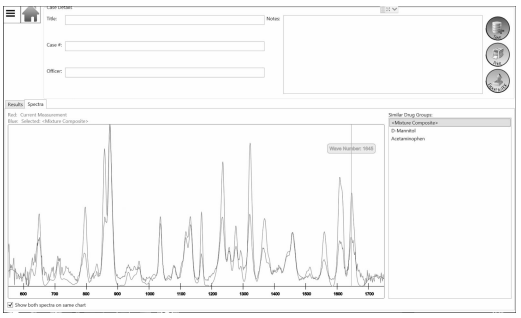
Analytical methods can be subdivided into three categories: unknown samples identification, express screening, and quantitative analysis.

Unknown samples identification	**Express-screening** (identification) of known samples		Known samples quantitative analysis
	with sampling	without sampling: through packaging and / or at-line quality control	
Standard applications			
Forensic science, mineralogy, art / artefacts attribution	Industrial labs (pharmaceuticals, polymer, chemical, others), products quality control	Quality control (raw materials, input, intermediate and final products); counterfeited products detection	Scientific and government labs, R&D, counterfeited products detection

Unknown Samples Identification

Each substance has its own unique Raman scattering spectrum that can be used to identify it. This can be achieved by comparing substance's Raman spectrum against a spectrum from a spectra libraries. There are several hundred thousands of inorganic compounds and tens of millions of organic compounds. In order to make an effective search in spectra libraries, it is recommended to choose respective libraries only (e.g. pharmaceuticals or polymers, petrochemical products or minerals). The software then matches a spectrum from an undefined sample against known spectra in a library. Hence, identifying the most likely candidate.

Below are some of the most common use cases.

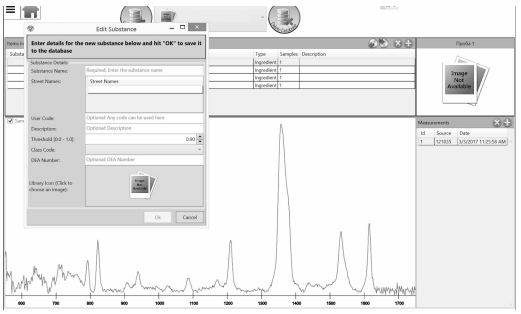


Acetaminophen spectra example

Express Screening of Known Samples

Express screening is used for quality control purposes in industrial production (e.g. quick identification of a large number of identical samples). In that case, a screening sample's spectrum compared against user-defined reference spectra.

Coda Devices' software enables end-user to create custom reference spectra libraries out-of-the-box.



Creating a user spectral library

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Mixture Analysis

The identification of mixtures' components is a more complex task. Coda Devices' software can quickly identify components as well as their relative percentage values in a mixture. For a successful mixture analysis components' spectra should significantly differ from each other and component should contribute no less than 10% to overall mixture's volume. Up to four components and their percentage values can be determined if these conditions are met.

A longer measurement time is required for components with lower concentrations. For example, 10 times longer time is needed for identifying a component that contributes only 3% to mixture's volume.

Separation of components with overlapped spectral lines is possible with the use of extra spectral data processing software.

Identification of four components in a mixture in less than 15 seconds

Quantitative Analysis

Intensity of spectral lines is proportional to the concentration of the respective substances in the sample. Due to this, the Raman method can be used for quantitative analysis, i.e. of concentration values determination. Quantitative analysis is used for the quality control in order to confirm that the substances concentrations are in the specified concentration range. For quantitative analysis calibration samples with known concentrations of analytes are prepared. It is necessary that the values of calibration samples are evenly distributed over the possible measurement range, and the range of their values is wider than the intended value of the measured concentrations.

RAMAN SPECTROSCOPY ADVANTAGES

Among the methods of chemical composition analysis (e.g.: nuclear magnetic resonance spectroscopy, mass spectrometry, infrared spectroscopy, etc.), Raman spectroscopy is the closest to infrared (IR) spectroscopy. Both Raman and IR spectra are similar with the only difference in the intensity of lines. In both cases, in the spectra reflects vibrations of atoms and groups of atoms in molecules. Frequencies of these vibrations correspond to the position of lines in the spectrum. Hence, frequency and spectrum type will change based on the molecular structure that comprises it. Thus making it possible to identify a chemical compound.

The most important advantages of Raman over IR spectroscopy are:

1. no need to prepare a sample. Hence, avoiding associated errors and significantly reducing time of analysis.
2. the possibility to take measurements through transparent packaging (e.g.: plastic bag, blister, test tube, etc.)
3. take measurements of aqueous solutions without the use of ultra thin liquid cells

Measurement through transparent packages

Compared to near infrared (NIR) range spectroscopy, Raman spectroscopy can drastically save your time and effort. NIR spectroscopy (i.e. 15,000 cm^{-1} – 4,000 cm^{-1} spectral range) shares with Raman method advantages listed above. However, unlike NIR, Raman spectral lines are analytical (i.e. their intensity is proportional to the concentration of substances). Therefore, calibration of the quantitative analysis using Raman spectroscopy require less than five reference samples. Meanwhile in NIR spectroscopy same calibration typically requires as few as tens samples. Thus, Raman spectroscopy can decrease calibration time by a factor of 10.

Moreover, in Raman spectroscopy, the compound identification is carried out using standard databases. While NIR method requires the creation of user's libraries. Hence, Raman spectroscopy also saves time and effort needed to create custom libraries.

Overall these advantages determine applications for Raman spectroscopy. High throughput of samples is possible due to a fast analysis. No need for trained professionals, since samples can be measured without a special preparation. Resources can be saved by avoiding breaking the initial package during quality control, thanks to the possibility of measuring through a transparent package.

Raman spectrometers can operate in warehouses and production facilities to ensure quality control of raw materials and final products, including standard size packaging (e.g. bags, packs, etc.). Raman method allows identification of counterfeit products, analysis of samples through a blister or clear glass vials, and identification of components in aqueous solutions.

CODA DEVICES PRODUCTS

CDI 1BT Bench-top Raman Spectrometer

CDI 1BT is specially built for use in laboratories. It measures the spectra of solid, liquid, gel and powder samples.

Select CDI 1BT to identify unknown substances or run an express analysis, conduct quality control or quantitative analysis of raw materials as well as final products. Optionally, CDI 1BT can be equipped with a PC, additional spectral databases and analytical software, vials and sample holders (e.g.: test tubes, tablets, etc.).

CDI 2 Handheld Raman Analyzer

CDI 2 handheld analyzer is ergonomic and easy to use. You are only one push away from identifying a sample. Results are ready in less than 15 seconds. CDI 2 weighs less than 6.5lb / 3kg and takes advantage of USB and Bluetooth connectivity.

CDI 2 is the right choice for quality control tasks, identification of unknown samples, use in outdoors, warehouses, production areas, and transport terminals. CDI 2 portability allows analysis of standard size samples eliminating the need for breaking initial packaging in order to take smaller samples. CDI 2 is also good for express screening with high-throughput of samples thanks to less-than-15-seconds standard measuring time.

CDI 1M Mobile Field Lab

CDI 1M combines the quality of a benchtop Raman spectrometer with ruggedness, portability, and autonomy needed for field work.

CDI 1M is specially built with the law-enforcement use in mind. It can quickly identify unknown substances like narcotics, prescription drugs, explosives, poisonous, etc. CDI 1M is equipped with a battery for 10-hours autonomous use and enclosed in a protective case capable of surviving even the harshest environments.

Specification

- weight and dimensions: 11kg / 24.25lb, 45 x 29 x 10.5cm / 18 x 11.4 x 4.2in
- battery time: 10 h
- charging from home or car socket
- operating temperature range: -10°C – +40°C / 14°F to 104°C
- typical measurement time: less than 15 s