Application Note

KEYWORDS

- Mid-IR region
- Overtone bands
- Ocean MZ5 spectrometer

TECHNIQUES

- Absorbance
- Vibrational spectroscopy

APPLICATIONS

- Chemical discrimination
- Food and flavorings analysis
- Environmental research

Why Choose Mid-IR Spectroscopy?

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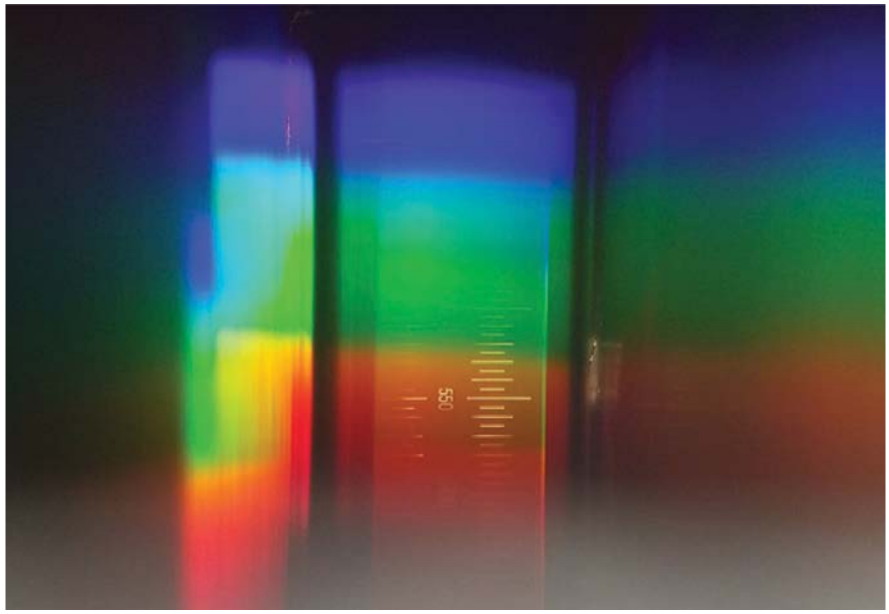


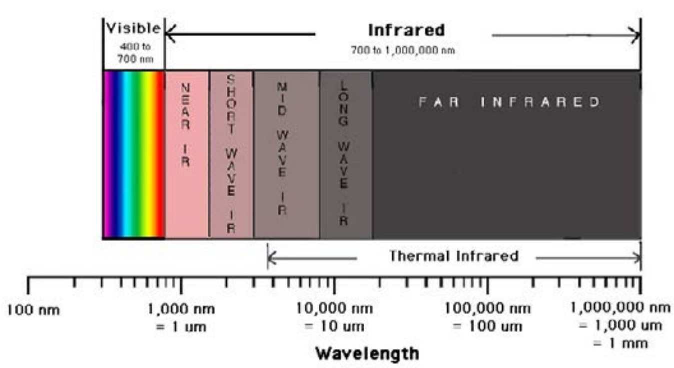
The power of spectroscopy is its ability to provide detailed information by measuring the interaction of electromagnetic radiation with a sample. The absorption/transmission, emission and scattering of electromagnetic radiation provide a wealth of information for determining sample composition and concentration, molecular and atomic structure, molecular interactions, sample identification and more. The information gleaned from spectroscopy measurements depends on many factors including the frequency of electromagnetic radiation used to probe the sample. In this technical tip, we discuss mid-infrared (mid-IR) spectroscopy and the applications where mid-IR is most useful.

Infrared Spectroscopy

Unlike radiation from the ultraviolet (UV) (~190-400 nm) and visible (~400-800 nm) regions of the electromagnetic spectrum, energy associated with radiation from the IR region is not high enough to excite electrons to higher energy levels. Instead, IR energy excites vibrational motions in the covalent bonds in molecules. Depending on the complexity of the molecule, a range of motions can occur including bending, stretching, scissoring, twisting and rocking in addition to rotational motion around the bonds of the molecule. The vibrational and/or rotational modes observed when IR radiation interacts with a molecule are specific to the chemical structure of the molecule being measured.

The infrared part of the electromagnetic spectrum is typically separated into three distinct regions based on the frequency of the IR radiation relative to the visible spectrum (~400-800 nm).

- Near-IR region: 12500-4000 cm^{-1} (~800-2500 nm wavelength) – closest to the frequency of visible light
- Mid-IR region: 4000-400 cm^{-1} (~2.5-25 µm wavelength)
- Far-IR region: 400-10 cm^{-1} (~25-1000 µm wavelength) – farthest from the frequency of visible light



Source: Global System Science

The detection of molecular vibrations and rotations that occur when samples absorb IR light is called vibrational spectroscopy. Near-IR, mid-IR and Raman spectroscopy are commonly used vibrational spectroscopy techniques. The vibrational modes measured when IR energy is absorbed by a molecule depend on the energy of the radiation interacting with the molecule. Overtone/harmonic and combination bands are excited by the higher energy in the near-IR (and visible) regions while lower energy mid-IR radiation excites the fundamental vibration bands. These fundamental vibrations arise from the simplest vibrational modes of the molecule and are stronger than the overtone and combination bands resulting from the fundamental vibrations. For this reason, spectra arising from fundamental vibrations are much cleaner, resulting in a unique fingerprint for the sample, which can be used for identification.

In the case of the far-infrared, the low energy of the radiation in this region makes it useful for rotational spectroscopy of inorganic molecules.

When is Mid-IR Spectroscopy Used?

The interaction of mid-IR radiation with a given sample provides a spectral fingerprint useful for identification of the sample. The mid-IR spectrum results from the absorption of specific frequencies of mid-IR radiation based on the chemical structure of the sample. For this reason, the peaks and troughs in a mid-IR spectrum are very specific to the sample measured. This makes mid-IR spectroscopy well suited for a wide range of applications involving materials identification and characterization from the analysis of fuels to detection of food contaminants and counterfeit materials. These applications and many others benefit from the fundamental bands measured with mid-IR, which yield a higher intensity, less convoluted spectra than the overtone and combination bands measured with near-IR and visible radiation.

Mid-IR spectroscopy is widely used by researchers and educators for basic and applied research and for teaching labs in physics, chemistry and biomedical courses. Here is a review of common applications of mid-IR spectroscopy:

Energy Technologies

As the world explores alternate energy sources and ways to reduce the environmental impact of fossil fuels, detailed fuel characterization and testing are required to ensure optimum performance and reduce environmental impact. Mid-IR spectroscopy can be used, to analyze FAME (fatty acid methyl ester) content in biodiesel, to test octane levels in fuel, to evaluate oil and lubricant degradation and to confirm the presence of fuel additives like ethanol.

Industrial

The specificity and non-destructive nature of mid-IR spectroscopy make it great for use in industrial settings including chemical and pharmaceutical production. In these industries, inbound raw materials must be tested to confirm identity. In addition, the product must be measured throughout the production process to ensure final product quality. In other industries, mid-IR is used for quality assurance to detect defects in finished products.

Industrial

With the advent of precision agriculture techniques to improve crop yields and decrease waste, mid-IR spectroscopy is used for soil characterization and to measure the content of constituents like antioxidants in agricultural products. Mid-IR is a great technique for feeding the consumer's desire to know more about the food they are eating including safety and quality. Mid-IR measurements are also very useful for confirming critical parameters like alcohol and sugar content.

Environmental Monitoring

With the current emphasis on protecting the environment, mid-IR spectroscopy is a great option for detecting soil and water contaminants including fuels and fuel products. Mid-IR spectroscopy is also used for airborne analysis to detect contaminant levels and to monitor high risk areas for environmental contamination.

In these and the many other applications using mid-IR spectroscopy, spectral analysis is based on two major regions in the mid-IR spectrum. Vibrations of the functional groups within the sample occur in the Functional Group Region from 4000-450 cm^{-1}. The much more spectrally complex Fingerprint Region from 1450-500 cm^{-1} provides a unique spectral region for the identification of samples.

Mid-IR versus Near-IR

Near-IR and mid-IR vibrational spectroscopy are widely used techniques with their own strengths and weaknesses. Both techniques require no sample preparation and provide non-destructive analysis but they both have attributes that make them better for certain applications.

Near-IR spectroscopy provides higher energy to the sample, but the spectra are composed of weaker overtone and combination bands, resulting in more complex spectra with overlapping absorption bands. Mid-IR spectroscopy measures fundamental vibrational bands related to the functional groups in the sample. These fundamental bands give clean spectra ideal for determining sample composition and for the identification of samples using their unique mid-IR fingerprint. Near-IR spectroscopy does offer an advantage in terms of sampling techniques with the ability to make reflection measurements in addition to the absorption and transmission measurements typically used for mid-IR spectroscopy.

In terms of sampling, near-IR spectroscopy enables more representative sampling of a larger volume of sample by rotating it throughout the measurement. This makes near-IR a good option for inhomogeneous samples and trace analysis.

Mid-IR spectroscopy, on the other hand, works best with smaller volumes of homogeneous samples making trace detection much more difficult.

Ocean MZ5 ATR-MIR Spectrometer

The Ocean MZ5 is a compact, fully integrated ATR-MIR spectrometer with measurement capabilities from 1818–909 cm^{-1} (5.5-11 μm). Ocean MZ5 comprises a sample interface, light source, detector and software, and provides a fast, convenient alternative to traditional FTIR spectroscopy.

Ocean MZ5 makes it possible to take on application challenges involving samples with distinct mid-IR absorption characteristics. This includes detection of food adulterants and contaminants, determination of oil grade and quality, and analysis of alcohol purity.

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