

Raman and FTIR Spectroscopy

Complementary Technologies for Chemical and Explosives Identification

Introduction

First responders faced with an unknown chemical substance have a number of immediate challenges, including choosing the most appropriate technology to assess the situation. Response tools for solid and liquid chemical identification include Thermo Scientific™ FirstDefender™ analyzers, based on Raman spectroscopy, Thermo Scientific™ TruDefender™ analyzers, based on Fourier Transform Infrared (FTIR) spectroscopy, and Thermo Scientific™ Gemini™ analyzer, which incorporates both lab-proven techniques in a single handheld instrument.

In both FTIR and Raman spectroscopy, the instruments acquire a spectral fingerprint of an unknown substance, and then compare the collected fingerprint against a reference library. Both methods are lab-proven, precise optical technologies offering distinct advantages in specific applications. Used together, FTIR and Raman spectroscopy provide a broader range of unknown substance identification—and better protection for the responder and the community.



Optical Techniques for Chemical Identification

FTIR and Raman spectroscopy measure the interaction of energy with the molecular bonds in a sample of an unknown material. FTIR measures how much light is the remaining energy from the original light source after being passed through the substance. In comparison, Raman measures the energy that is scattered after being excited by a laser.

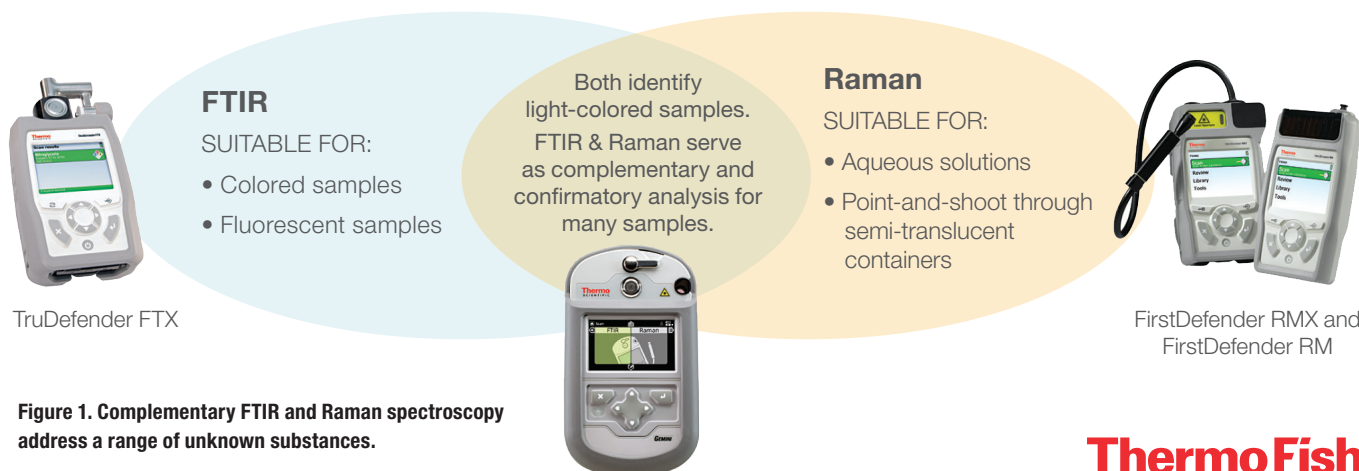
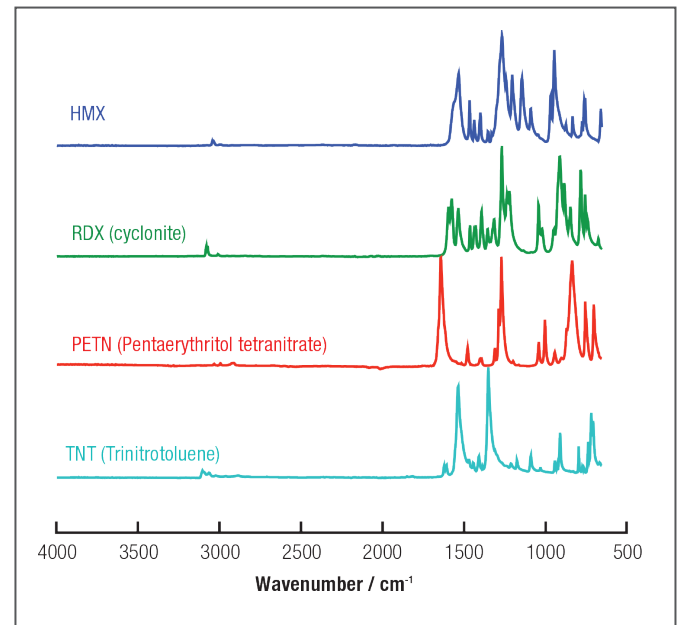


Figure 1. Complementary FTIR and Raman spectroscopy address a range of unknown substances.

FTIR Spectroscopy

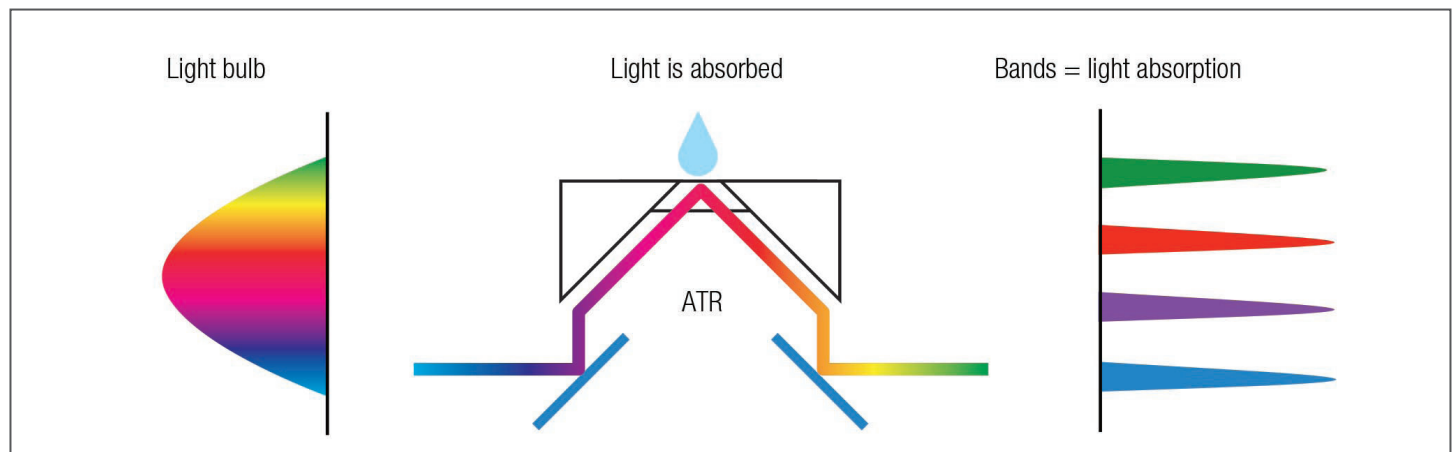
FTIR is an absorption spectroscopy technique, where mid-infrared light is passed through the sample. Some wavelengths may be absorbed while others merely pass through the sample unaffected. Specific molecular bonds absorb a specific amount of energy and these losses of energy correspond to the peaks returned in an analysis. FTIR absorptions provide outstanding and easily interpretable results for many substances. FTIR spectroscopy is best used as a primary analysis technique in the following scenarios:

- **Colored Substances:** Highly effective in identifying unknown solids and liquids of various pigmentations including industrial dyes, pigments and oils.
- **Fluorescent Materials:** Many colored samples produce optical noise called fluorescence during Raman sampling, which can obscure the spectral fingerprint of the substance. FTIR spectroscopy is ideal for fluorescent samples since it measures absorption of light, effectively eliminating this identification challenge.



FTIR spectra of select explosive compounds.

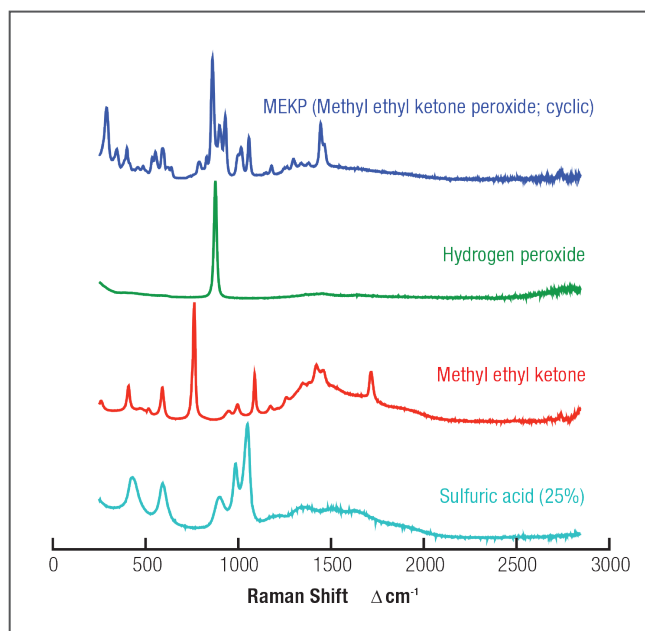
FTIR Spectroscopy



Raman Spectroscopy

Raman is a vibrational spectroscopy technique where a single wavelength laser is focused on a sample. The laser excites the bonds of a molecule, which generates measurable scattered light to identify the material in question. Raman is a highly effective method for reliable identification of an unknown substance based on its underlying chemistry. Raman spectroscopy is best used as a primary analysis technique in the following scenarios:

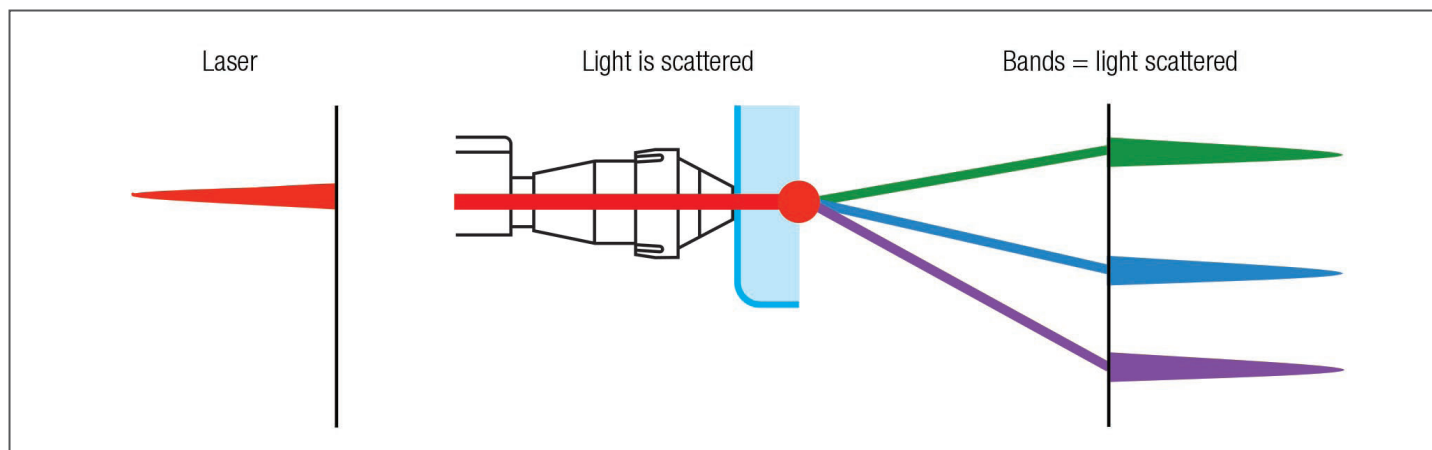
- **Sealed Containers:** As an optical technique, FirstDefender Raman spectrometers can operate in a point-and-shoot mode and analyze substances contained in transparent and translucent containers. This eliminates the need for direct contact with potentially hazardous unknowns. The integrated vial mode can also be used to analyze materials in standard colorless and amber glass vials.
- **Aqueous Solutions:** Raman spectroscopy virtually disregards water in samples (because of the very weak Raman signal) and is able to provide superior identification of potentially threatening materials in aqueous solutions.
- **White or Light Colored Powders:** Raman spectroscopy excels at the identification of white and light powders as these typically have very strong measurable Raman signals.



Raman spectra of select chemicals.



Raman Spectroscopy



FirstDefender Analyzers: Raman Spectroscopy

FirstDefender analyzers enable rapid, accurate identification of unknown chemicals directly in the field. At 1.8 pounds (800g), FirstDefender RM analyzers are designed to meet the demanding requirements of elite military personnel and civilian first responders, with a large, vivid display for ease of use by operators wearing bulky protective gear. FirstDefender RMX analyzers expand this capability with a fixed probe, allowing users to scan in hard-to-reach areas and to use scan delay. FirstDefender RMX analyzers can also be mounted on select tactical robots using the RS232 port and an integration kit.



TruDefender Analyzers: FTIR Spectroscopy

Using FTIR technology, TruDefender analyzers complement the FirstDefender product line to maximize in-the-field coverage of unknown chemicals, including explosives, toxic industrial chemicals, precursors and more. TruDefender FTX analyzers weigh 3.12 pounds (1.41kg) and are rugged enough to withstand the rigors of field use. The TruDefender FTXi instrument adds to this core functionality by providing a direct link to incident command or reachback support through embedded mobile phone technology.



Gemini Analyzers: Integrated Raman and FTIR Spectroscopy

Leveraging the strengths of dual technologies, Thermo Scientific Gemini analyzers are the first to integrate both Raman and FTIR in a single, rugged handheld instrument. Weighing 4.2 pounds (1.9kg), Gemini analyzers can be easily transported into the hazard zone, providing more comprehensive capability



Lab-Proven Techniques, Complementary Solutions

Two of the most widely-adopted technologies for identification of unknown solids and liquids are Raman and FTIR spectroscopy. The degree to which a substance responds to each technology is dictated by its unique molecular structure, with some responding extremely well to FTIR analysis and others being better suited to Raman. Thermo Scientific chemical identification tools were designed to leverage the power of each technique to maximize coverage of a broad range of unknown substances. When used alone, each technology quickly provides the analytical results needed to evaluate and identify unknown substances for safe remediation. When used together, TruDefender, FirstDefender or Gemini analyzers can serve as confirmatory techniques, providing a more comprehensive identification for greater confidence in response.

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