Analyze This:
Raman Spectroscopy for Explosives ID

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When dealing with an unknown chemical substance, explosives techs are faced with a number of immediate challenges, including deciding the best approach and tools for a situation. While detonate in place is one possible remediation protocol, this destroys evidence and may release other chemical hazards in the process. Collecting and transporting a sample is problematic due to potential instability and toxicity of the unknown substance, and the time required for transport and analysis. Because of these challenges, analyzing a substance in place when possible enables a technician to take appropriate precautions to protect themselves and the community.

For field analysis, some technologies such as x-ray, vapor/particulate analyzers and wet chemistry have been used extensively for years and are well understood within the EOD community. More recently, advances in optics, computing power and miniaturization—along with a narrowing gap between chemical hazards and explosives hazards—have led to an increase in use of spectroscopy for explosives identification. Proven in the lab for decades, some Raman and FTIR spectrometers (including those from Ahura Scientific) are now lightweight, handheld and rugged for field-based identification. While Raman and FTIR are complementary techniques and both are useful for explosives applications, this article will focus primarily on Raman spectroscopy. An article discussing FTIR for explosives in greater depth will follow in a future issue of The Detonator.

With Raman spectroscopy, a laser is focused on the sample of interest and the reflected light is collected by the instrument. While most of the light is reflected at the same wavelength as the original laser (called Rayleigh scatter), a small portion of the light is scattered in a very specific manner (Raman scatter) based on the molecular composition of the chemical, as shown in Figure 1. This scattered light forms a unique Raman spectrum, much like a fingerprint, which is then compared against a library of reference samples in order to identify the substance.

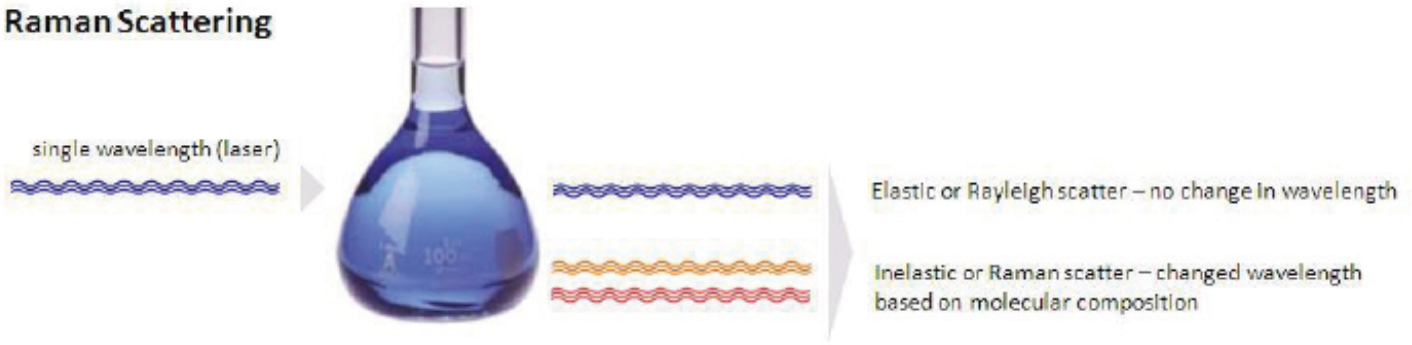

Figure 1

Figure 2 shows Raman spectra for several explosives and baking powder. You'll note that the spectra have very sharp peaks and can be distinguished despite some underlying chemical similarities. This high selectivity is important so a technician can confidently know what substance is present – for example TNT or picric acid – and therefore take the correct action to deal with the material and render the scene safe.

Raman offers both tactical and practical advantages over other identification techniques:
Analyze through sealed containers: As an optical technique, Raman spectroscopy is capable of identifying substances in sealed translucent or semi-transparent containers. Given the instability and potential sublimation of many homemade explosives, this offers great safety benefits to the technician. This is particularly advantageous when dealing with potential liquid explosives typically contained in sealed bottles.

Rapid results directly in the field: By bringing the instrument to the sample, rather than transporting the sample to a

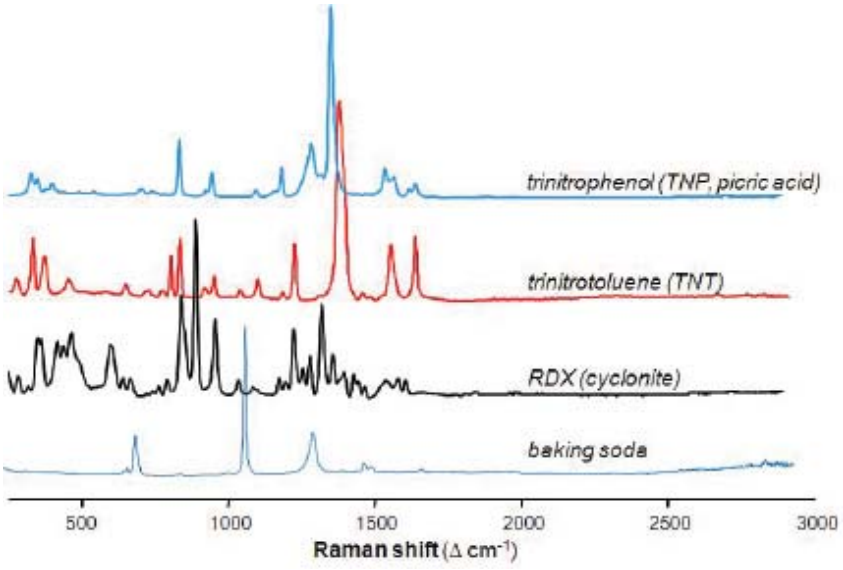

Figure 2

lab for analysis, response time is greatly decreased and a scene can be cleared more quickly. At the recent Republican National Convention, a FirstDefender Raman spectrometer was used by the St. Paul PD Bomb Squad to quickly analyze a suspicious package left at a vehicle screening point. By using this technology, the package was cleared with minimal impact on the screening area. [Source: The Detonator, Vol. 35, No.6, Page 36]

Non-destructive testing maintains forensic evidence: Unlike wet chemistry—or in an extreme example, detonation—Raman spectroscopy has no impact on the physical characteristics of the sample. If a substance is deemed safe, it can then be handled with the appropriate disposal procedures. Even if it's decided to detonate the substance after analysis, the analysis record including the specific collected spectrum is maintained for evidentiary purposes.

Many potential explosives found in the field will be mixtures, sometimes due to incomplete chemical processing during homemade explosives production or as a function of manufacturing for many military explosives. For example, many homemade explosives may contain common household precursors as well as a primary or secondary explosive component. Also, depending on the country of manufacture, C4 may be primarily RDX or may also contain some quantity of HMX. Whether mixture analysis is conducted automatically with software algorithms or manually via spectral subtraction, a technician can only understand the full scope of the threat when they understand as many components of a mixture as possible. Raman spectroscopy's inherent specificity is very beneficial for mixture analysis.

The FirstDefender Raman spectrometer is used to analyze an unknown chemical through the glass without touching or moving the sample.

Of course, there's no silver bullet; all technologies have limitations and drawbacks. Since Raman relies on reflected light for identification, dark substances which absorb a great deal of light are better suited for an alternate technology. Smokeless powder and dark-colored detasheet are the types of samples not amenable to Raman analysis. It's the color—not the chemistry—that causes the issue.

Highly fluorescent materials can also be problematic for Raman spectroscopy, though software algorithms from Ahura Scientific are designed to address this challenge. Fluorescence appears as a broad and nondescript curve on a spectrum, as compared to the sharp characteristic peaks of a Raman signal. This "noise" can slow a reading and make difficult to determine the molecular fingerprint of the sample.

During the past three years, Raman spectroscopy has emerged as an important part of the response toolkit. Used globally by military and civilian bomb squads and EOD teams, it adds another layer of safety and actionable information for use in response to unknown substances.