



# Vibrational Spectroscopy for Identification and Discrimination of Explosives and Common Household Materials

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## ABSTRACT

In the context of terrorist activity, both improvised and commercial explosives may be used but they are typically not clearly labelled and it is extremely difficult to identify explosives based on their physical appearance alone. In particular, they may physically resemble innocent common materials such as foodstuffs or cleaning materials. Here we discuss the use of vibrational spectroscopy as a means of identifying not only explosives but also explosives precursors and harmless materials which might be encountered in searches of potential for bomb factories. Previous literature has emphasized the value of identifying explosives and precursors, here we consider the advantages which vibrational spectroscopy may provide in identifying common household materials.

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## I. INTRODUCTION

Ever since the discovery of high explosives in the 19th century, terrorist and insurgent groups have relied on the use of Improvised Explosive Devices (IEDs) to propagate their campaigns. Instrumental methods for identification of explosives and precursors are an important component in the effort to counter terrorist threats and there are established methodologies for identifying suspect materials using laboratory based systems and simpler instruments at fixed sites, such as airport security stations. The detection technology typically needs to evolve in response to changes introduced by terrorist groups who are often forced to become innovative in their improvisation and modification of 'Home Made Explosives' (HMEs). This becomes particularly acute when the terrorist campaign is at a high tempo, and when it requires large IEDs such as car bombs or Vehicle Borne IEDs (VBIEDs). As the ingredients or precursors of these HMEs gain widespread use, the state will tend to regulate the materials in question.

Taking Northern Ireland as a Case Study, in the early 1970s, the Provisional Irish Republican Army (PIRA) at the start of their terrorist campaign, whilst using commercial and military explosive such as TNT in small IEDs, predominantly used sodium chlorate and nitrobenzene (known as 'Co-Op' mix) as a main charge in large car bomb VBIEDs. The sale of sodium chlorate, in the form of weed killer and nitrobenzene, in the form of chemical solvent, was strictly regulated by the government of Northern Ireland, resulting in the decline in the use of this HME recipe. PIRA then developed ammonium nitrate based explosive mixtures using agricultural fertiliser as the main source of this oxidizer, principally due to its ready availability in this rural region. The fuels used in the ammonium nitrate mixtures have included aluminium powder (AN-AL), diesel fuel oil (ANFO), nitrobenzene (ANNIE), and sugar (ANS). Attempts have been made to regulate the role and nitrogen contents of ammonium nitrate based fertiliser, starting in 1974, which has made its use of fertiliser as an HME precursor more problematic for the terrorist but still an oxidizer of choice that remains attainable and effective.

These examples highlight the why there is a general need for instrumental methods for identification of homemade explosives that can readily evolve in response to new threats. These would also preferably be portable and sufficiently easy to use to allow field use, since this would both allow ad hoc screening and facilitate identification of locations where explosives and/explosive devices are being prepared. Vibrational spectroscopy has significant potential in this area since both infra-red and Raman spectrometers suitable for field use have been developed.[1]-[4] These systems are typically equipped with spectral libraries containing examples of the spectra of standard explosives and automatic searching of unknown spectra against these libraries should, in principle, allow the composition of the sample to be identified. The libraries can also be updated as required in response to new threat materials Library identification is made possible by the fact that every chemical compound has a unique spectral signature since the

intensities and positions of the peaks it contains are determined by the number and strength of the bonds within the compound, which by definition are different for different compounds. However, what is less often discussed is the fact that although each spectrum is expected to be unique, the spectral differences between chemically similar compounds will be small since chemically similar compounds will mostly have similar bonds. Here we discuss how these effects influence the potential for identification of both explosive and harmless household materials since both these are expected to be encountered in settings where explosive devices are manufactured in or near domestic settings.

## **2. EXPERIMENTAL**

All infrared spectra were recorded using a Bruker Alpha FTIR which was fitted with an ATR sampling system. In use, a few mg of sample were placed on the ATR crystal and pressed into onto the surface using the integral mechanical lever. Raman spectra were recorded with a Delta-Nu ReporteR spectrometer or Ocean Optics IDRaman Mini 2.0, both of which 785 nm excitation as a compromise between the need to avoid fluorescence by using a wavelength as far to the red of the visible range as possible and the need to remain within the high quantum efficiency range of the silicon detector.

## **3. Results and Discussion**

Some samples lend themselves well to both IR and Raman analysis. For example, Figure 1 compares the IR and Raman spectra of the commercial explosive PETN. In the figure it is obvious that both forms of spectroscopy give rich spectra with numerous bands but that the spectra are quite different from each other due to the different selection rules which apply to each. Nonetheless, simple library searching will give an immediate match to either of these spectra. However, many samples do not yield high quality spectra of this type due to interference from other effects such as fluorescence or water absorption. This is true for both explosives and to an even greater extent, household materials.

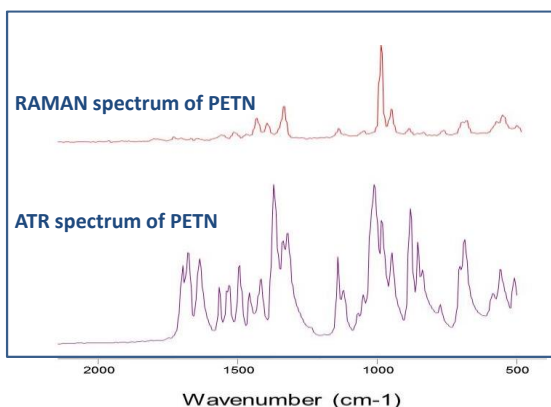


Figure 1. An example of a commercial explosive sample, PETN, which gives high quality IR and Raman spectra.

Figure 2, for example, compares the Raman spectra of common household materials. The spectrum of the curry powder shows significant background fluorescence which masks the weaker Raman signals under a broad intense but featureless signal. Such adventitious fluorescence is a common feature in the Raman spectroscopy of unpurified real world samples which may contain small

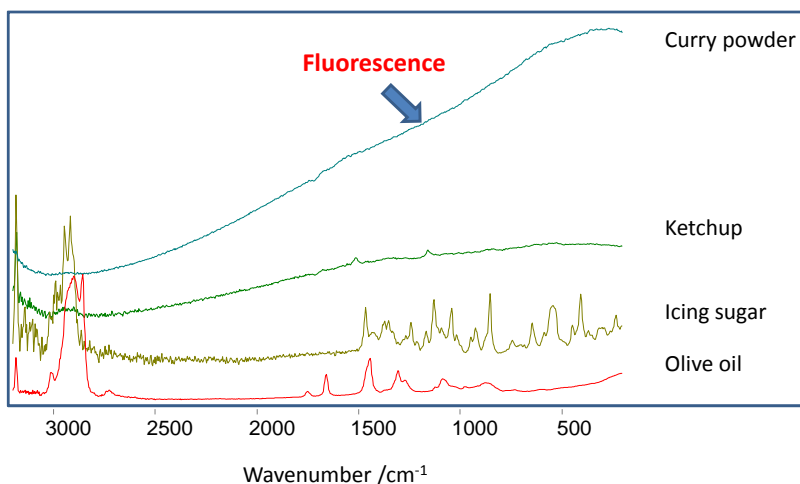
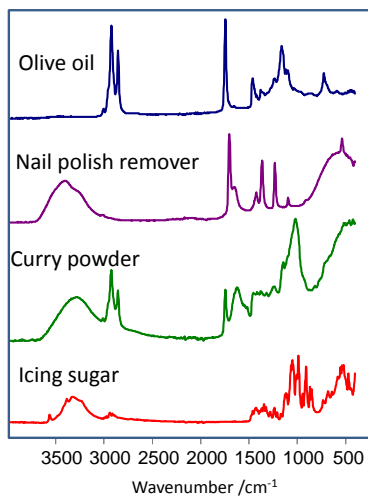


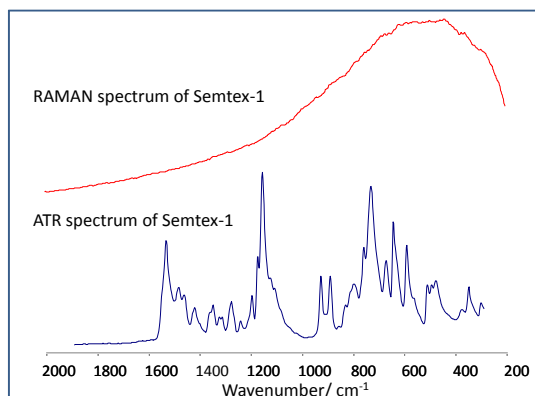
Figure 2. Raman spectra (785 nm excitation) of common household materials. The spectrum of the curry powder was significantly more intense than the other spectra shown and was rescaled.

amounts of highly fluorescent materials. Infrared spectroscopy does not suffer from this problem, as illustrated in Figure 3, which shows IR spectra of the same materials shown in Figure 2.



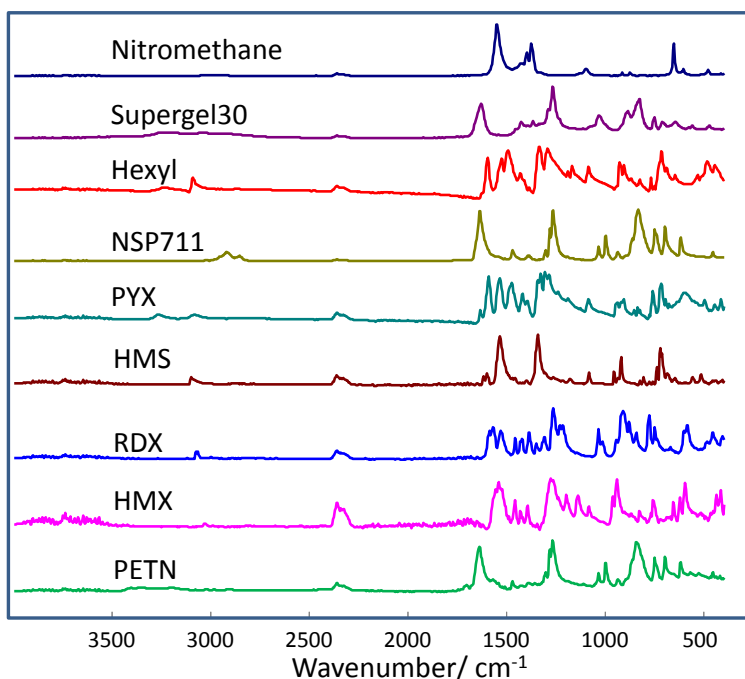
**Figure 3. The infrared ATR spectra of the 4 samples whose Raman spectra are shown in Figure 2.**

In this case all the materials give high signal-to-noise spectra with minimal background interference although it is important to note that substances with a high water content give poor IR spectra while the water gives minimal interference



**Figure 4. Raman and ATR-IR spectra of Semtex showing fluorescence interference in the Raman spectrum.**

in Raman spectra. We have found in initial tests of 33 samples that 50% gave useable Raman spectra but highly coloured materials were problematic. Conversely, IR worked well for most highly coloured samples but failed with wet samples. Overall >90% of random samples gave useful spectra from at one least one of the techniques.



**Figure 5. ATR-IR spectra of a selection of explosives.**

Similar results were found for explosives, in that a significant number of samples were fluorescent, as shown for Semtex in Figure 4. Conversely, useable IR spectra were obtained for the vast majority of samples since the explosives and precursors had low water content, as illustrated in Figure 5.

It is clear that the IR spectra of the explosives show significant differences and it is therefore not surprising that spectral matching of these materials with library data was 100% accurate.

## 4. Conclusions

In a simple choice between IR and Raman spectroscopy for explosives identification the problem of fluorescence means that IR has a higher success rate than IR for substance identification. However, when the sample set is expanded to

include common household substances which often have a moderate to high water content, Raman spectroscopy's advantage of low water interference becomes important and a combination of both IR and Raman spectroscopy is required in order to have achieve a high identification rate.

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