

## A104 High Resolution Fourier Transform Spectroscopy for the Discrimination of Lab Grade Explosive Precursors and Their Shop-Bought Equivalents

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After attending this presentation, attendees will have an understanding of the application of high resolution Fourier Transform infrared spectroscopy for the characterization and discrimination of explosives precursors and how this can be used to inform and develop explosives detection systems.

This presentation will impact the forensic science community by demonstrating the suitability of high resolution Fourier Transform mid-infrared spectroscopy for the discrimination of different brands of shop-bought materials which have the potential to be used as explosive precursors. The work will also explore the ability of high resolution Fourier Transform mid-infrared spectroscopy and chemometric analysis of the resultant data to distinguish shop-bought materials from each other and from their lab grade counterparts.

The development of accurate and sensitive explosives detection systems is an area of significant and substantial growth. The challenges facing the development of such systems are diverse, and, as a result, there are multiple approaches to solving them. However, one factor is constant through these approaches: in order to detect a compound; it must first be characterized in order to identify distinguishing features that can then be targets for detection.

While many explosives detection systems provide the ability to detect an explosive compound when part of an improvised explosive device, another approach is to further expand the capacity to detect explosive precursors as a means of identifying sites of illicit explosives manufacture, or those involved with the production of explosive materials. This has the potential to continue to prevent the production of explosive devices, and identify the bomb makers. Detecting the manufacture of explosive devices prior to completion has the demonstrated and significant benefit of making seized materials safer for the security services to handle and greatly reduces the risk to the public. An increased knowledge of explosive devices as the materials involved will affect the breakdown of the explosive material and may be detectable as this occurs. For example, a hydrogen peroxide-based explosive such as Triactetone Triperoxide (TATP) will emit hydrogen peroxide vapor which can then be detected.

With the increase in the use of homemade explosive devices, there is continued desire to characterize the precursors of these materials. Due to the nature of these explosives, many of the precursor materials are available "off the shelf" and have many legitimate uses. However, the majority of these "off the shelf" chemicals will not be in a pure form, with various additives present to aid in the materials legitimate use. For example, acetone in nail polish removers is combined with perfumes, emulsifiers, emollients, aversive agents, and colorings. This work investigates whether it was possible to discriminate both between lab grade chemicals and their "off the shelf" counterparts, and between different brands of "off the shelf" materials using high resolution Fourier Transform spectroscopy and statistical analysis.

Previous work has demonstrated that high resolution Fourier Transform mid-infrared spectroscopy paired with basic data analysis is a useful tool for the characterization of explosives and explosive precursors. While the information gathered via this technique is a useful resource in its own right, it is also able to directly inform the development of a quantum cascade laser-based explosives detection system.

High resolution Fourier Transform mid-infrared spectroscopy should be particularly suited to the task of discrimination, as the increased resolution allows the system to be capable of resolving minute spectral features. In addition, while the instrumentation is able to look at minute details, it is also able to cover the whole mid-infrared region so the technique can be considered information rich. The impact of the information produced with a spectrum can then be enhanced by statistical analysis of the data.

This presentation reports the result of the comparison of lab grade liquid explosive precursors with "off the shelf" materials. The comparison and discrimination is made both by visual comparison of the spectra produced and also through statistical analysis of the data.

Explosives Detection, IR Spectroscopy, Statistics