Detection of Homemade and Commercial Explosives, Taggants, and Precursors With the Vocus Chemical Ionization Mass Spectrometer

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Introduction

Fast, sensitive detection of explosive substances is a crucial requirement for law enforcement, military, and security experts. Tools that can detect civilian, military, and homemade explosives and their synthetic precursors are useful for counterterrorism efforts, controlling environmental contamination, mitigating illicit trade, and research such as assessing canine training aids.

Sensitive detection of trace explosives is challenging. Explosives that have very low volatility (do not evaporate easily) emit very little residue into the air and are therefore difficult to detect without direct or close-proximity sampling. Some explosive samples may include contaminants or residual precursor chemicals mixed with the explosive compounds of interest. Detection of these ancillary chemicals may be used to indicate the presence of an explosive, but this indirect approach requires assembling a large database of samples to ensure reliable detection.

The TOFWERK Vocus chemical ionization (CI) TOF mass spectrometer is an extremely sensitive chemical detector which excels at detecting traces of carbon-containing compounds in air. Through partnership with explosives testing facilities, TOFWERK characterized the performance of the Vocus CI-TOF for measurement of select explosive samples. The Vocus CI-TOF directly analyzes air in real-time – reporting data instantaneously with no required sample preparation - and each explosive sample was measured simply by holding it in front of the detector's inlet. Irrelevant chemicals detected in the background laboratory air were subtracted to reveal the chemical signature of each sample.

Figure 1 shows several common explosives, precursors, and taggants organized by vapor pressure (vertically) and chemical composition

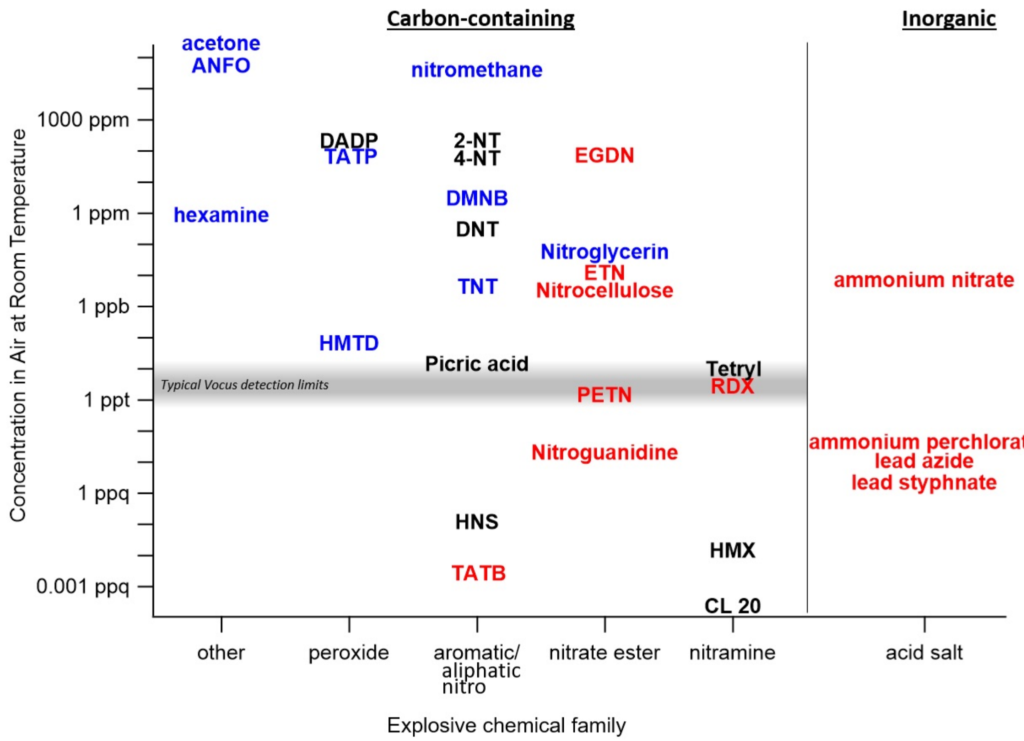

Figure 1 *Explosives and related chemicals arranged by volatility and chemical structure. Compounds with proven detection by Vocus CI-TOF are shown in blue, untested compounds in black, and undetectable compounds in red. Typical Vocus CI-TOF detection limits with 1-second measurement are indicated by the gray shaded area. The volatility of lead azide and lead styphnate is unknown but likely low.*

(horizontally). The types of compounds optimally detected with the Vocus CI-TOF include lightweight, highly volatile carbon-containing compounds in the upper left region of the diagram. Generally, this space overlaps with compounds detectable by dogs. Canine detection limits are difficult to determine, but evidence suggests they are in the range of 1 ppt to 500 ppt, depending on the compound, which is very similar to Vocus capability [1]. For comparison, conventional ion mobility spectrometers (IMS) used in airports have detection limits around 10 to 100 ppb, which is a thousand to ten thousand times less sensitive.

What the Vocus CI-TOF Reports When Measuring Explosives

Mass spectrometers, such as the Vocus CI-TOF, output “mass spectra” that show the abundance of chemical species having different molecular masses. Figures 2 though 6 show mass spectra measured by the Vocus CI-TOF when sampling different explosives for approximately one second. Each vertical peak in a spectrum represents the detection of a specific chemical species emitted by the sample. The height of the line shows the relative abundance of the chemical, and the bottom axis shows the molecular mass, which is used to identify the chemical species. The measured mass spectrum, the relevant “fingerprint” molecules, and the calculations to determine the intensity of the signal are incorporated into the detector software, making the routine procedure simple. The operator views only the detected intensity of the explosive odor over time, and optionally an indicator if the odor signal crosses a pre-determined threshold.

Easy-to-Measure Substances

Some substances are easy to detect: they have a high vapor pressure and are sensitively detected by the Vocus CI-TOF. The chemical signatures measured by the mass spectrometer include a small number of unique chemicals that are clearly related to the target substance. TATP, C4 taggant, and TNT are good examples (Figure 2).

The TATP and TNT molecules are sensitively and selectively detected by the Vocus CI-TOF. The taggant molecule included in C4, DMNB, is also easy to detect. The detector is so sensitive to these compounds that residual contamination from these species can be detected on surfaces days after the substance is removed: see our application note, “Realtime Detection of the Explosives TATP and HMTD.” In addition to the C4 taggant, the instrument also detects fragments of the polyisobutylene binder.

Other examples of easy-to-detect compounds, with high vapor pressure and simple chemical signatures, include hexamine, nitromethane, and acetone, although nitromethane and acetone have other sources and are not reliable indicators of the presence of explosives.

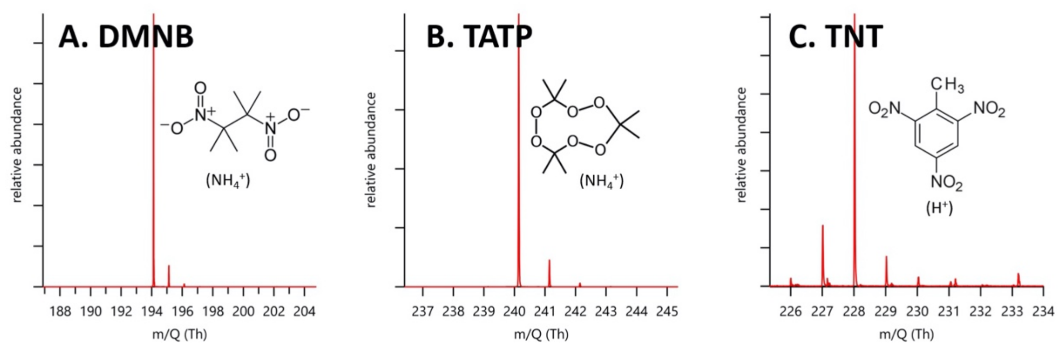

Figure 2 *A) detection of 2,3-dimethyl-2,3-dinitrobutane (DMNB) in C4 explosive, B) detection of TATP, C) detection of TNT.*

Substances That Can Be Clearly Detected Using Their Chemical Fingerprint

Some explosive substances can be recognized by a complex combination of many chemicals. Match heads have been used as an improvised explosive because they are easy to obtain in bulk. It is possible for the detector to identify them using a pattern of nitrogen-containing volatile chemicals (Figure 3A). ANFO (ammonium nitrate fuel oil) has a characteristic pattern of hydrocarbons from the fuel oil (Figure 3B).

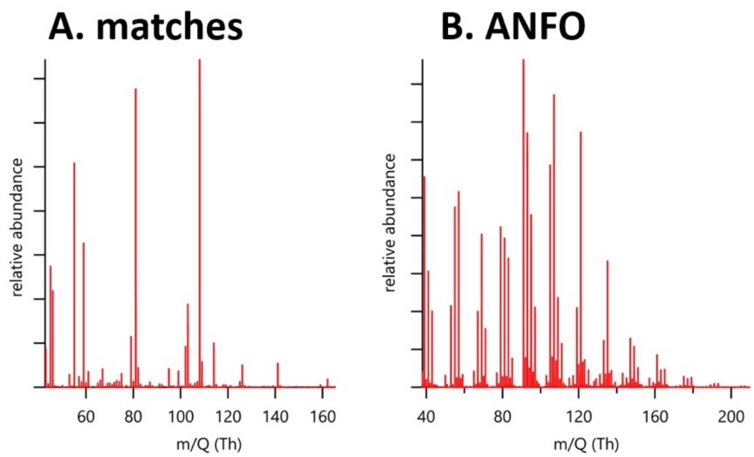

Figure 3 *A) Detection of ground match heads. B) Detection of fuel oil.*

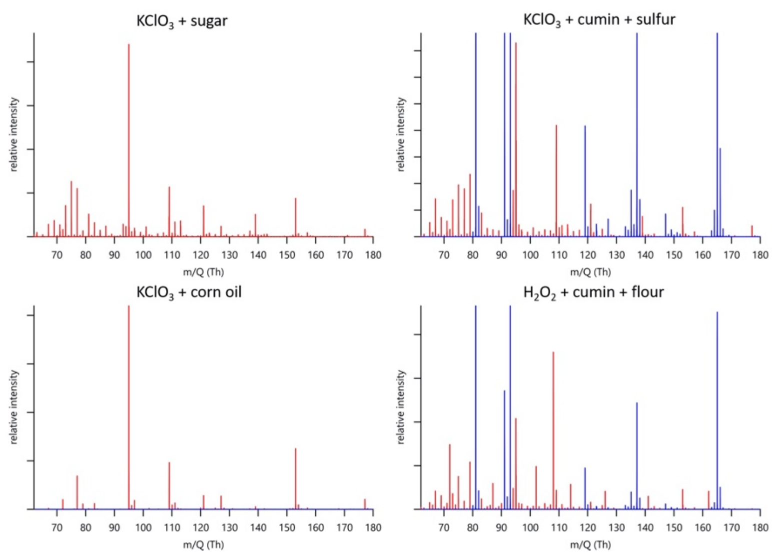

Figure 4 *Chemical fingerprint of potassium chlorate and concentrated hydrogen peroxide mixtures. Note the characteristic molecules at 95, 109, 121, 139, and 153. In the mixtures including cumin, the molecules derived from the cumin are highlighted in blue.*

Potassium chlorate and concentrated hydrogen peroxide cannot be detected directly, but when mixed with an organic substance such as flour, sugar, or corn oil, volatile organic compounds are emitted and can be detected (Figure 4). Improvised explosives using "black seed" or cumin are also extremely easy to recognize due to the presence of cuminaldehyde, a unique detectable aroma.

Difficult-to-Measure Substances

Some molecules are difficult to detect because of their low vapor pressure: only an extremely small amount of the explosive evaporates into the air and can be sampled by a

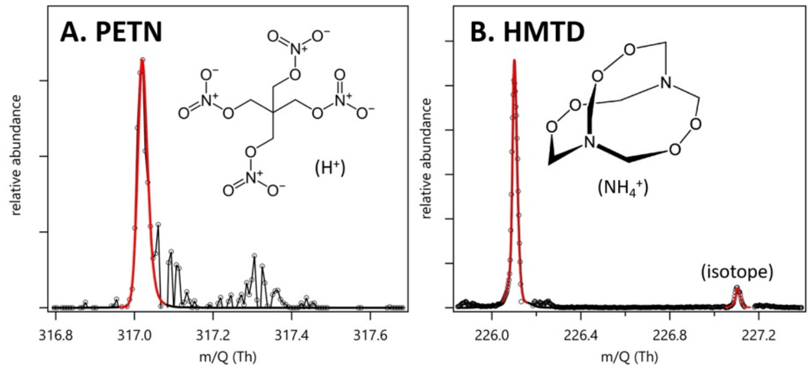

__Figure 5__ A) detection of PETN. B) detection of HMTD

detector. For example, the PETN molecule can be detected by the Vocus CI-TOF (Figure 5A), but the vapor pressure is so low that it is not realistic to detect a PETN-bomb by directly sampling air. The vapor pressure of HMTD is slightly higher, and HMTD can be detected in ambient air, but it is difficult to do so (Figure 5B). Sampling using a swab, followed by heating to evaporate the explosive residue into the detector inlet could provide a reliable method to detect HMTD, PETN, and other low-volatility chemicals such as nitroguanidine, RDX, HMX, tetryl, and PGN.

Some explosive mixtures have main components that cannot be detected by the Vocus CI-TOF, or would need a swab sampler to detect, but nonetheless emit carbon-containing compounds that are detectable. These compounds could be contaminants or residues left over from manufacture. These could be used to alert to the presence of explosives, but would require building a large database including samples of diverse origin. Examples including black powder, double base smokeless powder, sulfur powder, and DBX-1 are shown in Figure 6.

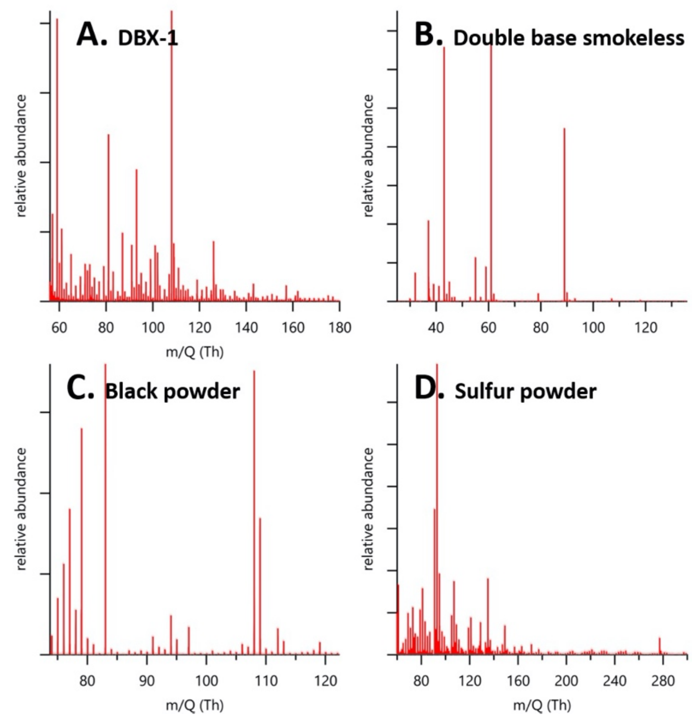

Figure 6 A) Volatiles detected from DBX-1. B) Volatiles detected from double base smokeless powder. The largest signals are related to organic acids and ethyl acetate. C) Volatiles detected from black powder. D) Volatiles detected from sulfur powder.

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References

[1] Oxley, J. C., and Waggoner, L. P., Chapter 3 - Detection of Explosives by Dogs, Ed. Marshall M., Oxley, J. C., Aspects of Explosives Detection, Elsevier, pp 27-40, 2009.