Rapid and Sensitive Detection of Explosives and Trace Residues

Felipe Lopez-Hilfiker

TOFWERK, Thun, Switzerland

Law enforcement agencies require tools to quickly and safely identify explosives and residues. Chemical ionization mass spectrometry (CI-MS) is a sensitive, real-time gas-phase analysis technique that is well equipped to detect a variety of explosives at trace levels. CI-MS, as implemented with the Tofwerk Vocus CI-TOF mass spectrometer, can measure molecules with a wide range of chemical properties and vapor pressures. Ambient air is introduced directly into the chemical ionization region of the Vocus, and the generated ions are robustly detected by the TOF mass analyzer, leading to extremely fast response times with no sample preparation.

Realtime Detection of Trace Triacetone Triperoxide (TATP)

In close proximity sampling, time response and sensitivity are critical for high-speed screening. The Vocus CI-TOF can measure multiple times per second and has response times of fractions of a second for many organic compounds. One such compound is the explosive triacetone triperoxide (TATP), which has been used in several high-profile terrorist attacks and is of particular interest to law enforcement agencies. Figure 1 shows the real-time, fast detection of TATP. A subject carrying a canine training aid (a small, highly dilute sample of TATP) walked several times in front of the Vocus CI-TOF detector. Ventilation directed the low-concentration plumes of TATP to the detector inlet. Each detection of the TATP "threat" is visible as a sharp spike.

![Figure 1. Fast, real-time detection of TATP. A human subject carrying a small amount of TATP walked several times in front of the Vocus CI-TOF detector. Ventilation directed the low-concentration plumes of TATP to the detector inlet. Each detection of the TATP “threat” is visible as a sharp spike.](image-url)
Figure 2 Detection of residual TATP inside a contaminated package. A cardboard box was briefly exposed to TATP, then left unsealed for 20 hours. The air inside the box was periodically sampled with the Vocus CI-TOF. The measured concentration of TATP decreases over time but remains well above the instrument detection limit.

of the Vocus detector at a 2-meter distance. Direction of the plume towards the inlet ensured reliable detection. Each passage is immediately visible in the monitored, TATP-specific ion as a sharp spike with a width of a few seconds. The sensitive, rapid response measurement of TATP in plumes is realized even with only trace emissions of TATP, making this detector suitable for mobile platforms.

Explosives leave residues behind on clothing, packaging, and other surfaces. The high sensitivity and selectivity of Vocus CI-TOF allows real time residual explosive vapor analysis. Figure 2 shows the measurement of residual TATP on the inside of a cardboard box over a period of nearly 1 day. The cardboard box was exposed to the canine training aid for 45 seconds. Less than 50 μg of vapor was exposed to the interior of the box surface. The box was left unsealed and was periodically measured with the Vocus CI-TOF using a flexible inlet line. Even after nearly 20 hours, TATP can be detected at nearly 100 times the instrument detection limit.

Sensitive Detection of Low-Volatility Explosives

The Vocus CI-TOF can also be used to detect explosives with even lower vapor pressures. The vapor pressure of the explosive is critical, as this is what determines the gas-phase concentration above the solid or liquid. Vocus CI-TOF detection limits are in the parts-per-trillion (pptv) and parts-per-quadrillion (ppqv) range for common explosives. Hexamethylene triperoxide diamine (HMTD) is a highly explosive organic compound with low vapor pressure. This means that the detection could be more influenced by isobars and other compounds present in air. Detection after large dilution is much more challenging. A low vapor pressure explosive such as HMTD requires excellent sensitivity to detect at all.
HTMD vapors from a canine training aid, released at room temperature, were measured with the Vocus CI-TOF. Figure 3 shows that HMTD is immediately observed in room air when the sample is held near the inlet. A quantitative understanding of the ion-molecule reaction chemistry allows the determination of the HMTD vapor concentration at a few tens of pptv. Use of swab samples and thermal desorption could allow the detection of even lower volatility explosives.

**Contact**

mail@tofwerk.com

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