Sicrit technology

Application Note

Fast and Direct Detection of Explosives using SICRIT®-MS

Summary

- Soft ionization of relevant explosives
- Direct MS measurement of samples without chromatography
- Easy automation of sampling using PAL autosampler
- Adaptable to any LC-MS

Introduction

The detection of explosives and explosive-related compounds is a high-priority tasks in recent years for homeland security and counter-terrorism applications. There has been a lot of research in the field of mass spectrometry regarding selectivity, sensitivity, and portability.

Taking advantage of the SICRIT® soft ionization source, this ambient MS technology may contribute to new MS-based approaches for fast and direct analysis of explosives.

The SICRIT® ionization source can be „plug & play“ interfaced with the atmospheric pressure inlet of any LC-MS system and therefore offers the possiblity for easy adaption to the specific performance requirements.

The miniature flow-through design of the source enables direct „sniffing“measurements in room air without any need for consumables, e.g. noble gases.

These SICRIT® key features suggest diverse application scenarios: Not only fast and direct screening of solid and liquid samples (e.g swabs) at a stationary site can be performed, also mobile sniffing and online-detection tasks could be realized. E.g. thinking on walk-through portals and explosive sniffer dogs as used in airport security, SICRIT® could present a versatile alternative for real-time monitoring of critical infrastructures.

Experimental Setup

Aim of this preliminary study was to investigate SICRIT® soft ionization regarding its ionization potential for relevant explosives.

Most of the relevant compounds can be ionized in negative mode due to their nitro functional groups. Therefore, the compounds listed in Table 1 were analyzed in negative mode with exception of TATP, which was analyzed in positive mode.

For analysis, 1 µL of a 3 ppm solution mix of Tetryl, TNT, FOX-7, PETN, HMX , RDX and TATP (each 3 ng absolute) were directly injected into the SICRIT® GC/SPME module (200°C, carrier gas: humidified N_2) and analyzed. For sample injection, a PAL3 RTC system (CTC Analytics) was used.

MS measurements were performed on a LTQ Orbitrap XL system (Thermo Fisher) in negative or positive full scan mode (mass range 50-500 m/z, resolution of 30.000 FWHM). The plasma conditions of the SICRIT® source were set to 1.5 kV at 15 kHz in all experiments.

Table 1 - Investigated explosive compounds

Compound	Sum formula	Dominant product ion species	Measured mass of product ion (m/z)
Tetryl	$C_7H_5N_5O_8$	$[M-NO_2]^-$	241.0210
TNT	$C_7H_5N_3O_6$	$[M-H]^-$ $[M-NO]^-$	226.0099 197.0198
FOX-7	$C_2H_4N_4O_4$	$[M-H]^-$ $[M+NO_3]^-$	147.0156 210.0112
PETN	$C_5H_8N_4O_{12}$	$[M+NO_3]^-$	377.9999
HMX	$C_4H_8N_8O_8$	$[M+NO_3]^-$	358.0238
RDX	$C_3H_6N_6O6$	$[M+NO_3]^-$	284.0225
TATP	$C_6H_{12}O_4$	$[M+NH_4]^+$	240.1432

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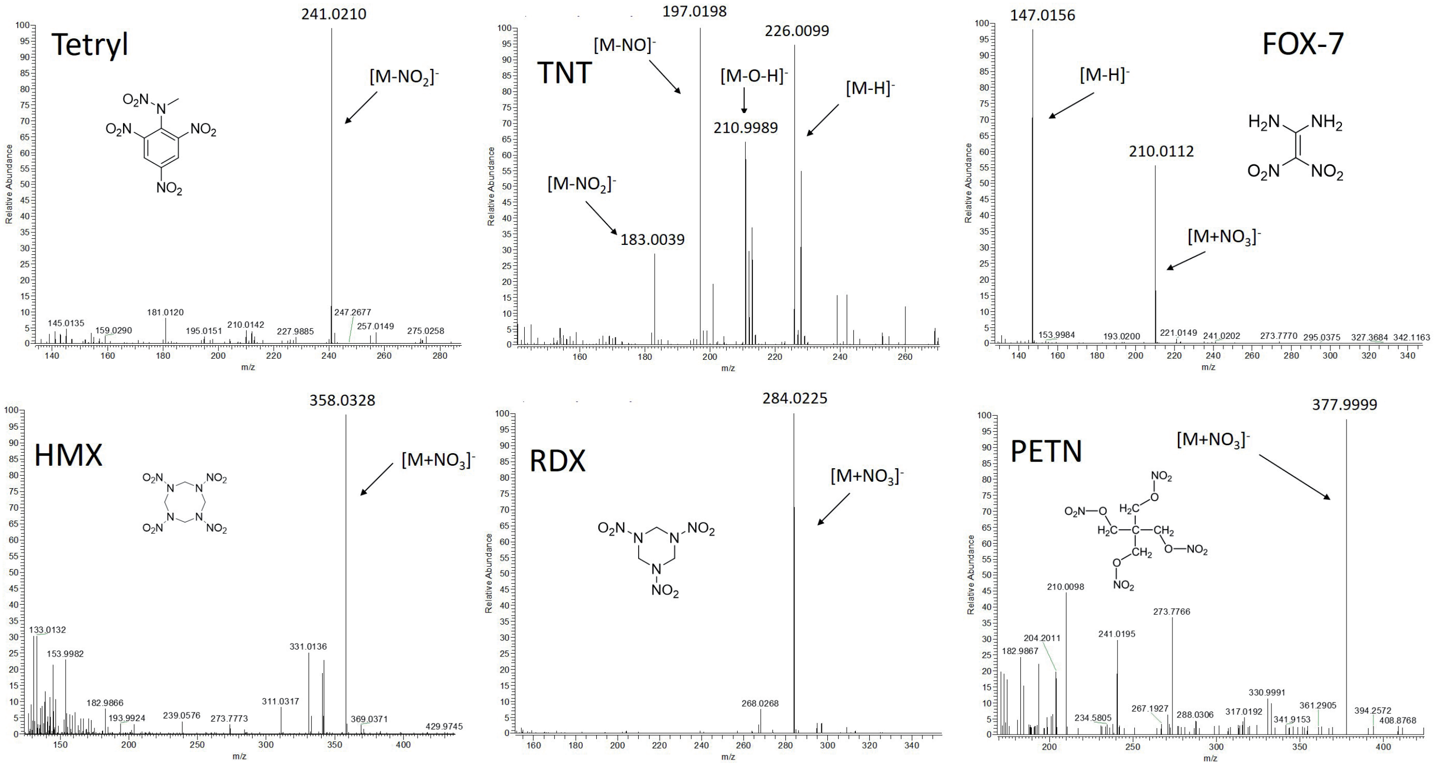

Figure 1 - Full MS spectra of investigated explosives (3 ng absolute) in negative mode, obtained on LTQ Orbitrap XL (Thermo Fisher).

Results

All of the investigated explosive compounds could be successfully and softly ionized by SICRIT®. Using high-resolution, dominant product species could be assigned to the compounds. As listed in Table 1, the spectrum of Tetryl shows $[M-NO_2]^-$ as dominant product ion species, whereas the other compound spectra are dominated by $[M+NO_3]^-$ adduct product ions (see Figure 1).

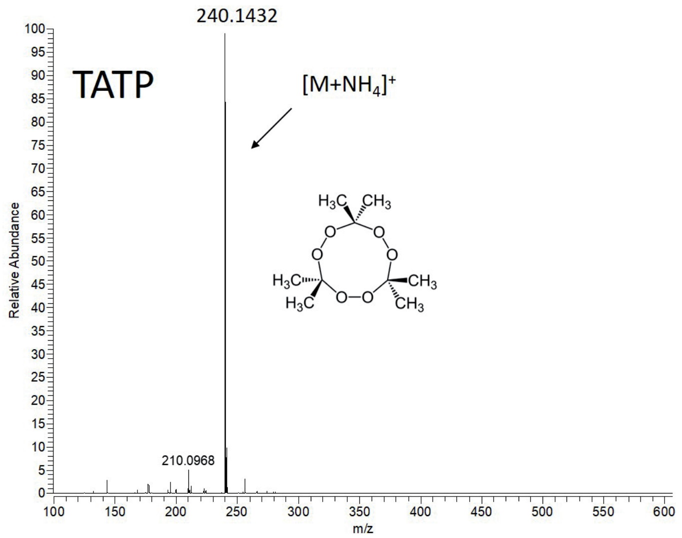

Figure 2 - Full MS spectra of TATP (3 ng absolute) in positive mode, obtained on LTQ Orbitrap XL (Thermo Fisher).

In case of TNT, $[M-NO]^-$ is present as main species besides $[M-H]^-$.

In positive mode, TATP could be efficiently ionized and detected as $[M+NH_4]^+$ adduct species.

The obtained spectra demonstrate the soft ionization potential of SICRIT® which can be used for definite identifcation of the explosive compounds.

Conclusions

The presented data show efficient and soft ionization of relevant explosives using SICRIT®. These promising results suggest further investigation regarding sensitivity in combination with MS systems also suitable for fast, mobile, and in-field security applications. As some of the actual detection methods are struggling with a lack of selectivity and/or sensitivity, SICRIT® may contribute to new sensor solutions in this field, based on soft ionization-MS.

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