E48 Ambient Ionization Mass Spectrometric Detection of Homemade Explosives in the Presence of Precursors

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After attending this presentation, attendees will have a better understanding of how the concurrent mass spectrometric detection of homemade explosives and their precursors can be affected by factors such as competitive ionization and differences in chemical properties.

This presentation will impact the forensic science community by providing methods for the detection of homemade explosives in the presence of their precursor chemicals and other complex matrices. The presentation will also present methods to mitigate deleterious effects caused by the presence of precursor molecules.

Chemical analysis and detection of explosives is a well-explored area of forensic science in which numerous methods have been investigated. Techniques such as Gas Chromatography/Mass Sspectrometry (GC/MS), infrared spectroscopy, and colorimetric tests can all readily detect a wide range of explosives in both pure form and in complex matrices; however, the capabilities of one of the emerging techniques in forensic science, Ambient Ionization/Mass Spectrometry (AI/MS), has been significantly less researched due to the recent advent of the platform. Most work completed thus far, regarding AI/MS capabilities, has focused on the detection of pure compounds or common military-grade explosives in known matrixes. While it is essential to evaluate the performance characteristics of these techniques under controlled conditions, it is equally as important to investigate common homemade and improvised explosives. Two common classes of homemade explosives are sugar alcohol-based nitrate ester explosives, such as Erythritol Tetranitrate (ETN) and Xylitol Pentanitrate (XPN), and peroxide-based explosives, such as Triacetone Triperoxide (TATP) and Hexamethylene Triperoxide Diamine (HMTD). Since these compounds are typically homemade, it is crucial to understand their performance characteristics and potential detection issues both in pure form and in mixtures with their precursors.

This work focuses on identifying potential advantages and issues in the detection of homemade explosives when found in the presence of their common precursor chemicals using AI/MS platforms. The main platform investigated is Direct Analysis in Real Time Mass Spectrometry (DART®-MS). DART®-MS has been shown to rapidly and sensitively detect a number of explosive compounds from various classes with minimal-to-no-sample preparation. Utilizing a heated stream of helium metastable atoms, ionization of explosives rapidly occurs through either adduct formation, deprotonation, or protonation. One of the major benefits and drawbacks of the DART®-MS and AI techniques in general is the lack of a chromatographic separation prior to ionization and mass spectral detection. While this lends itself to rapid sampling times, it also may prove deleterious when complex mixtures are analyzed. Competitive ionization and differences in chemical properties can favor ionization and detection of one compound over another.

A number of sugar alcohol-based explosives were analyzed by DART®-MS as neat compounds and in the presence of their common precursors, sugar alcohols and nitric acid. Through analysis of these mixtures, it was found that competitive ionization does occur when these compounds are concurrently sampled. Relative affinity for free nitrate ions and differences in vapor pressures of the explosives and related sugar alcohols components can lead to diminished detection limits of the explosive component. Furthermore, extracted ion chromatographs of the mixtures highlight how different ionization pathways are preferred in the presence of different combinations of precursors, with adduct formation with free nitrates being the dominant pathway for both components. Studies have also been completed which focused on maintaining the sensitivity of the explosive compound by altering the chemical properties of the atmosphere near the sampling area, through dopant introduction. This work has shown that different ionization pathways can be emphasized depending upon the dopant species present. While current work has focused on sugar alcohol-based explosives, work is now continuing and will be presented on understanding peroxide-based explosives and their precursors as well as investigating additional AI/MS-based techniques such as Desorption Electro-Flow Focusing Ionization/Mass Spectrometry (DEFFI/MS).

Homemade Explosives, DART®-MS, Competitive Ionization