B103 The Detection and Forensic Analysis of Trace Fuel-Oxidizer Mixture Evidence by Infrared Thermal Desorption (IRTD) With Direct Analysis in Real-Time Mass Spectrometry (DART®-MS): Black Powders and Black Powder Substitutes

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Learning Overview: After attending this presentation, attendees will understand how coupling Infrared Thermal Desorption (IRTD) with Direct Analysis in Real Time Mass Spectrometry (DART®-MS) can be utilized to analyze and differentiate trace collections of fuel-oxidizer mixtures, specifically targeting black powder and black powder substitutes. Attendees will be presented with representative chemical signatures for these compounds at multiple points in the desorption profile, as well as their identification and discrimination based on multivariate statistics.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by introducing a unique analytical platform for the trace detection and forensic analysis of wipe-based sample collections, including both organic and nonvolatile inorganic species. The IRTD-DART-MS platform generates rapid and discrete heating ramps, allowing for near simultaneous detection of volatile organic species at lower temperatures and nonvolatile inorganic oxidizers at elevated temperatures. By combining the ability to rapidly identify the full range of chemical species in conjunction with multivariate statistics, this platform provides the forensic examiner a tool to generate high fidelity data for identification and differentiation of black powders and black powder substitutes.

The detection and accurate identification of trace evidence pertaining to homemade explosives remains imperative to the public safety and forensic science communities. Wipe-based sampling of surfaces remains a common method for the collection of trace evidence for further analysis. These sample collections can be chemically analyzed using a wide range of analytical techniques from *in situ* colorimetric detection to laboratory-based liquid chromatography mass spectrometry (LC/MS). Many existing techniques are hindered by targeting a single species or the need for extractions and lengthy analysis times. To combat these constraints, several platforms exist or have recently been developed and/or modified to enable the thermal desorption of target species directly from the wipe-based collection. However, these platforms often maintain a constant thermal desorption temperature, optimized for a specific target analyte or class of analytes. This aspect leads to difficulties in the detection and analysis of nonvolatile inorganic oxidizers found in fuel-oxidizer and self-initiating mixtures commonly playing an important role in homemade explosives as well as illegal or counterfeit fireworks.

To address these hurdles, an infrared thermal desorption (IRTD) platform was developed and coupled with the ambient mass spectrometry technique, direct analysis in real time (DART)-MS, through and enclosed T-junction interface. This coupling takes advantage of traditional ambient mass spectrometry benefits, including, rapid analysis at atmospheric pressure and no additional sample preparation, while introducing a novel mode for analyte thermal desorption. The IRTD platform enabled discrete and rapid (5s to 15s) heating ramps that reached the high temperatures (450°C to 550°C) needed for the thermal desorption of nonvolatile inorganic oxidizer species. The inherent temperature profile generated by the infrared emission allowed more volatile organic species to be thermally desorbed at lower temperatures without degradation or decomposition, followed by the thermally desorption of refractory inorganic oxidizers at elevated temperatures. IRTD-DART-MS demonstrated nanogram to sub-nanogram sensitivities for several common organic explosives and inorganic oxidizers as neat samples. The methodology developed for the detection of these nonvolatile inorganic oxidizers was deployed for the identification and differentiation of a range of black powders, black powder substitutes, and flash powders. These powders represent of class of fuel-oxidizer mixtures of forensic interest due to their abundance and availability as a low explosive or incendiary compound. Due to the diverse ion distributions generated by these complex mixtures, the multivariate statistical method, principal component analysis was employed for their identification and discrimination. In addition, the characteristic temperature programmed desorption achieved by the inherent temperature ramp was exploited for a level of separation of volatile and nonvolatile species. The IRTD-DART-MS and multivariate statistics demonstrated a unique platform enabling the direct identification and differentiation of trace fuel-oxidizer mixtures.

Infrared Thermal Desorption, DART®-MS, Black Powder Substitutes