Detection and Characterization of Chemical Attribute Signatures from Smokeless Powders by Dynamic Headspace Concentration and DART-MS

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Overview
- High throughput detection and characterization of chemical attribute signatures from energetic materials used in the creation of IEDs by DART-MS

Purpose:
- Rapidly sample and analyze traces of pre- and post-blast energetic materials used to charge IEDs by reducing sample preparation and analysis time
- Improve collection efficiency of trace explosive components using sorbent-coated screens
- Rapidly generate chemical attribute signatures (CAS) from smokeless powders

Introduction:
- Domestic terrorism involving the use of improvised explosive devices (IEDs) creates public concern resulting in a need to develop rapid methods for the identification of the explosive components in order to promptly provide investigators with answers
- IEDs may be constructed using military explosives but are typically designed from non-military components such as smokeless powder and black powder.
- Recent studies have shown how chemical attribute signatures can be used to differentiate different types of smokeless powders.
- Dynamic Headspace DART-MS was employed to demonstrate a high-throughput method requiring minimal sample preparation.

Methods:
- DART-Standard Voltage and Pressure (SVP) ambient ionization source interfaced to a ThermosQuest Finnigan LCQ Deca
- Smokeless powders from various manufacturers
  - Seven unburnt powders
  - Five burnt powders
- Dynamic Headspace
  - Powders were heated in Al paint cans sealed with modified lids
  - Temperature, time, and flow rate were evaluated
  - Headspace vapors were evacuated with a vacuum and concentrated onto Carboxapack X screens
- SRK glass fiber filters were used to filter incoming room air
  - DART He temperature: 200°C
  - Carboxapack X screens placed in Open Spot Quick Strip module
- Stabilizers and plasticizers were detected in positive ion mode
- Energetic materials were detected in negative ion mode
- Comparison with conventional GC-MS analysis

Dynamic Headspace DART-MS Method Development

DART-MS Method
- Sample Preparation: dynamic headspace concentration
- Sample size: 5 min per sample
- 110°C
- 3 L/min
- DART SVP coupled with a ThermosQuest Finnigan LCQ Deca ion trap MS
- He temperature: 200°C
- Analysis Time: 1.5 min per sample

GC-MS Method
- Sample Preparation: 2 flakes of powder dissolved in 1 ml acetonitrile
- 45 min to 1 hr or more
- Injection port: ~30 min on rocker/shaker
- GC: 790 GC with 5975 single quadrupole MS
- Injection port: ~30 min on rocker/shaker
- Analysis Time: 30 min per sample

Results

Positive Ion

Negative Ion

Comparison of DART-MS and GC-MS

Conclusions
- Chemical attribute signatures from smokeless powders were rapidly and successfully generated with dynamic headspace sampling and analysis by DART-MS
- Seven different smokeless powders were characterized and differentiated.
- Signatures from burnt powders were comparable to unburnt powders.
- This dynamic headspace DART-MS method offers and permits rapid sampling and analysis of smokeless powders.
- DART-MS provided additional signatures that cannot be detected by conventional GC-MS methods.
- Future directions: employ AnalyzAir®, an offline statistical software, to build models to characterize and differentiate smokeless powders based on the generated chemical attribute signatures.

References

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