AccuTOF-DART ®Analysis of Smokeless Powders

Introduction

Smokeless powders (Figure 1) are often used in improvised explosive devices. The formulations for smokeless powders vary between manufacturers and between brands from a given manufacturer; ingredients include energetics, stabilizers, plasticizers and deterrents. Chemical analysis of smokeless powders can provide valuable forensic evidence. Here we show that the AccuTOF-DART mass spectrometer can rapidly identify the organic components in smokeless powders and provide a chemical fingerprint that can be used to identify individual powder particles.

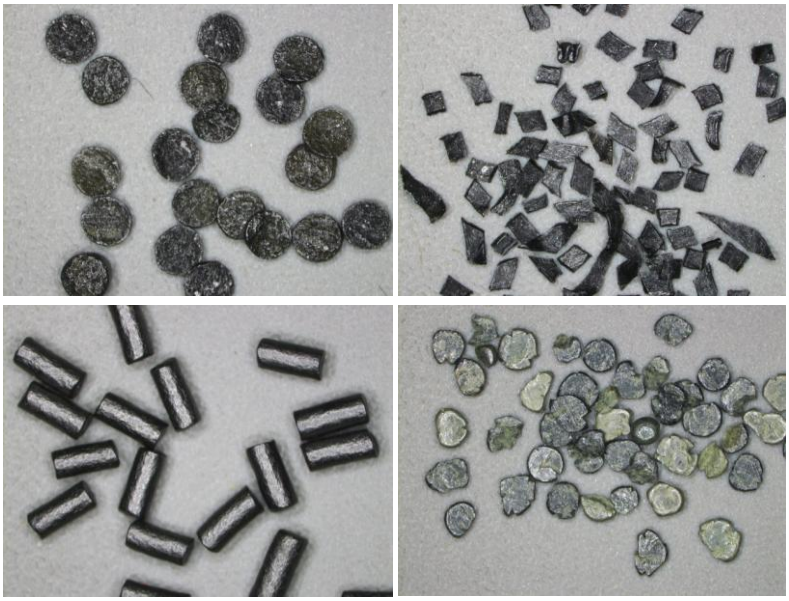

Figure 1. Several smokeless powders viewed under an optical microscope.

Experimental

The AccuTOF™ mass spectrometer was operated in positive-ion mode. Polyethylene glycol (PEG-600) was measured as a reference standard within each data file, but separate from the smokeless powder particle measurements. Individual particles sampled with vacuum tweezers were positioned in the DART gas stream for analysis (Figure 2). Disposable vacuum tweezers were constructed by passing a glass capillary through an Eppendorf pipette tip and inserting the pipette tip into a rubber hose connected to a low-vacuum pump. Data were acquired by using JEOL Mass Center software and mass spectra were processed by TSSPro3 software (Shrader Software Solutions, Detroit, MI).

Figure 2. AccuTOF-DART analysis of a smokeless powder particle.

The DART ion source was operated with a gas heater temperature setting of ≤200°C to avoid damaging or detonating the smokeless powder particles. Individual samples could be analyzed within seconds. As long as the gas heater temperature did not exceed 200°C, the samples were not consumed and could be examined or reanalyzed at a later time.

A list of target compounds commonly used in smokeless powders was created in a Microsoft Excel spreadsheet. The spreadsheet contained the names and elemental compositions of the target compounds. The target compound spread sheet was used by Mass Mountaineer software (www.mass-spec-software.com) to identify compounds in the smokeless powder mass spectra based upon exact masses and isotopic data. The Mass Mountaineer program also allowed us to create and search mass spectral databases created from the mass spectra of smokeless powder standards.

Results

The AccuTOF-DART mass spectra for several smokeless powders are shown in Figure 3a and 3b. The DART mass spectra show unique patterns of organic components typically detected as protonated molecules $[M + H]^+$. Because some samples from the same manufacturer showed the same organic components, but had different morphology, it appears that both morphology and DART analysis will be required for a unique identification of a specific powder.

Because labeled compounds were tentatively identified by solely by exact mass and isotopic data, the presence of isomers cannot be ruled out. Regardless, the mass spectra are reproducible and distinctive, making it possible to identify unknown particles by comparison against database spectra.

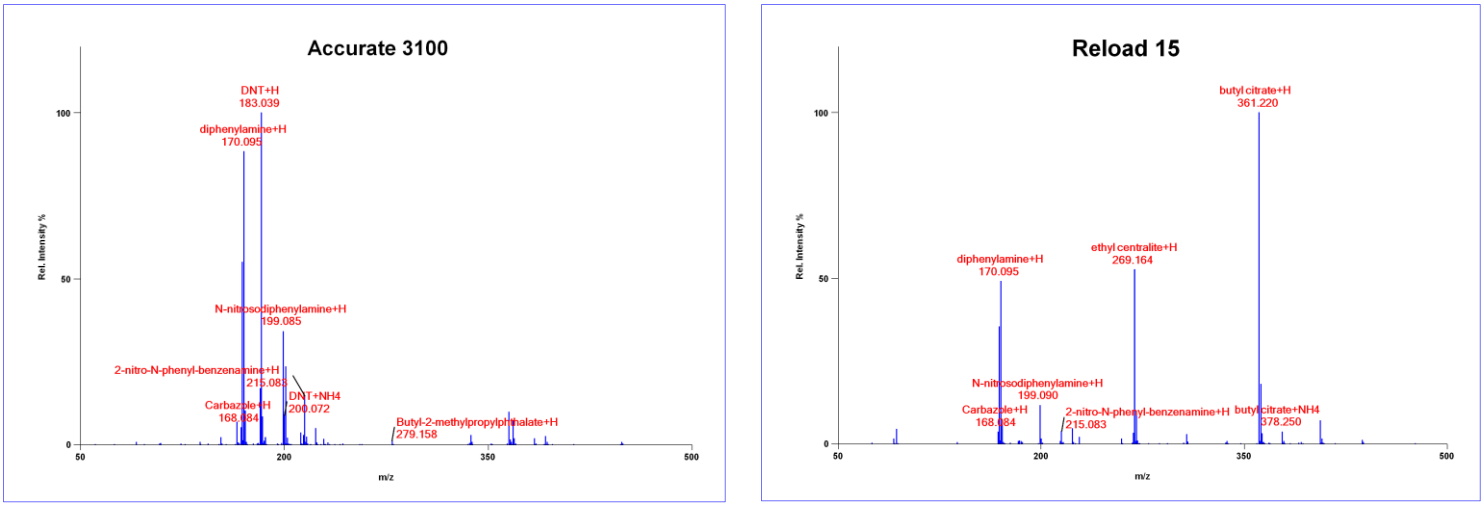

Figure 3. (a) AccuTOF-DART mass spectrum of an Accurate 3100 smokeless powder particle; (b) AccuTOF-DART mass spectrum of a Reload 15 particle.

Conclusions

The AccuTOF-DART mass spectrometer is capable of rapid fingerprinting of organic compounds in smokeless powders. Although further work needs to be done to expand the database and validate the method, the AccuTOF-DART mass spectra (in combination with particle morphology) offer a rapid and potentially nondestructive approach for the identification of individual smokeless powder particles.

Acknowledgement

We are grateful to John A. Meyers who suggested this work and provided background information and the initial set of smokeless powder samples that we analyzed at the 2008 Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (PittCon).