A147 Evaluation of Different Atmospheric Pressure Ionization (API) Sources for Use in Explosives Detection

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After attending this presentation, attendees will learn of the distinct ionization mechanisms for each of these sources and which is the most efficient for applications involving explosives detection in the field.

This presentation will impact the forensic community by comparing three atmospheric pressure ionization sources and providing a basis for choosing an adequate technique for the analysis of explosives in varied scenarios and crime scenes.

This presentation will discuss the use of atmospheric pressure ionization sources for the detection of the explosives, TNT, TNB, 1,3- TNB, 2,6-DNT, Tetryl, RDX, HMX, PETN, and NG. Attendees will learn of the distinct ionization mechanisms for each of these sources and which is the most efficient for applications involving explosives detection in the field.

The development of highly sensitive techniques capable of trace explosives detection and straightforward identification is increasingly desirable in the forensic community. There is a strong demand for methods able to perform field analysis of involatile and thermally unstable explosive compounds with rapid response time, and preferably without complicated sample preparation. API is a soft ionization technique that can be operated at atmospheric pressure and room temperature, making it possible to perform mass spectral detection of explosives in the field. Three API methods, atmospheric pressure chemical ionization (APCI), desorption electrospray ionization (DESI), and distributed plasma ionization source (DPIS), were evaluated to determine ionization mechanisms and ability to detect nine explosive compounds.

The APCI has already been developed and used to detect and analyze explosives under various conditions because of user-friendliness, high sensitivity, reliability, and its widespread availability, which enables detection in ambient environment. Recently, more API sources have been developed to meet the requirements of low detection limits, high- throughput, and portability, such as DESI and DPIS. APCI uses a corona discharge at atmospheric pressure and is mainly applied to polar compounds with moderate molecular weight up to about 1500 Da and generally gives monocharged ions. The DPIS is a type of direct ionization technique for mass spectrometry which is based on the production of a nonequilibrium plasma. This plasma is generated around one of the electrodes and is fairly easy to use at atmospheric pressure to generate analyte ions. DESI is conducted under ambient conditions by spraying untreated samples with ionized solvent droplets from a pneumatically-assisted electrospray. Desorption and ionization of the analyte occurs through interaction with the charged droplet or with impacting gas-phase ions generated by the primary electrospray. These three methods, with their different ionization mechanisms, were selected because they are potentially amenable to field measurement.

In this research, 2,4,6-trinitrotoluene (TNT), 1,3,5-trinitrobenzene (TNB), N-Methyl-N,2,4,6-tetranitroaniline (Tetryl), 2,6-dinitrotoluene (2,6-DNT), 1,3-dinitrobenzene (1,3-DNB), Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane (HMX), pentaerythritol tetranitrate (PETN), and 1,2,3-propanetriol trinitrate (NG) were selected for analysis by these sources based on their structural classes: nitroaromatic, nitramine, and nitrate ester, respectively. The explosive solutions were diluted in a solvent containing 65% methanol and 35% deionized water. Experiments were performed by employing an API/MS system, comprising one of the three API sources and a commercial ion trap mass spectrometer. Gas-phase explosive ions were generated by APCI, DPIS and DESI. Negative ion mode was generally chosen for detecting the deprotonated molecule $[M- H]^-$. However, addition of an organic acid or salt is necessary to form adduct ions for nitroamine and nitrate ester explosives, such as RDX, HMX, PETN and NG, because of their lack of acidic protons. In this research, approximately 0.1% of carbon tetrachloride was used as an additive to form stable adducts ions with nitramine and nitrate ester explosives. All solutions were diluted to a concentration of about 10 parts per million (ppm), as this is fairly realistic based on calculated explosive detection applications.

Atmospheric Pressure Ionization (API), Mass Spectrometry, Explosives

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