A10 Explosives Analysis Using Gas Chromatography/Mass Spectrometry

Randi S. George, BS, 705 S Gulph Rd, King of Prussia, PA 19406; Heather L. Harris, JD, 2401 Lombard St, Ste 1, Philadelphia, PA 19146; and Barry K. Logan, PhD, Center for Forensic Science Research and Education, 2300 Stratford Ave, Willow Grove, PA 19090*

After attending this presentation, attendees will be able to assess their current laboratory techniques for analysis of problematic compounds and determine if the GC/MS method will improve trace explosives identification for a wider variety of compounds in relation to their current methods.

This presentation will benefit the forensic science community by showing laboratory personnel how to adjust their GC/MS equipment for the clearest mass spectra of high explosive compounds and their isomers.

This research will demonstrate those highexplosive compounds that do not survive typical GC/MS conditions. It also presents a new database of compounds for GC/MS, including common high explosives and related compounds. Such a complete database of these compounds is difficult to find, making this a useful tool for any laboratory.

More laboratories use GC/MS than any other technology for analytical purposes. Gas Chromatography (GC) is advantageous in trace analysis as it has a high resolving power, resulting in more efficient separations, which lead to better identifications. Mass Spectrometry (MS) is an accurate and reliable detector with the capability of examining a broad range of compounds and identifying them with specificity. The combination of GC with MS allows for improved separation of complex matrices and specific identification of trace analytes.

The greatest obstacle when analyzing highexplosive compounds by GC/MS is the high reactivity and propensity of the compounds to decompose rapidly at high temperatures. At high temperatures, the explosive compounds decompose and their mass spectra contain ions that can be found in a wide variety of molecular decompositions, making it difficult to produce and identify a unique explosive compound. In addition to the temperature challenges, active sites can be found throughout the chromatographic system attracting these explosive compounds and binding with them. The explosive compounds become lost in the system and never appear in the MS source to produce a spectrum.

This research includes method development for the following compounds: Trinitrotoluene (TNT), Cyclotrimethylenetrinitramine (RDX), Cyclotetramethylene-Tetranitramine (HMX), Pentaerythritol Tetranitrate (PETN), Dinitrotoluene (DNT), and Trinitrophenylmethylnitramine (tetryl). Optimum inlet temperatures for each of these compounds were determined in an attempt to decrease the effect of the most common decomposition location.

Three main inlet temperatures, 250°C, 150°C, and 80°C, were tested with TNT, RDX, HMX, PETN, and Tetryl. Of these inlet temperatures, 250°C was determined to be optimum for PETN, 150°C for tetryl and RDX, and 80°C for HMX. TNT was not affected by differing inlet temperatures. Furthermore, tetryl's mass spectrum matched N-methyl picramide, a product of tetryl hydrolysis, which was expected from reports in the literature. RDX showed breakdown resulting in a lower level of m/z 76 present in the spectrum. Similar data was collected from a total of 35 compounds including high explosives, their isomers, plasticizers, and others found in the presence of explosives.

This research will benefit the larger community of law enforcement, military, and even industry by providing more options to laboratories for explosive analysis. Forensic explosive analysis can identify compounds in improvised explosive devices (IEDs) and land mines in war zones to properly identify explosive components in pre- and post-detonation situations. Explosive manufacturers and research facilities would benefit from improved analytical techniques to determine the quality of their product and to evaluate changes that occur to bulk materials in storage.

The benefits go beyond these communities; however, extending into the environmental and medical fields. Improved analysis will help identify environmental soil and water samples contaminated by runoff and erosion from blasting and storage sites at lower levels, so the problem can be remedied before permanent damage occurs. Along with proper extraction techniques, GC/MS is capable of isolating and identifying each specific compound at the trace levels at which these compounds will most likely be detected. The challenges associated with this research project, the solutions to those challenges, and the resulting mass spectra for high explosives and related compounds for compilation into a user-searchable database will be presented.

Explosives, Gas Chromatography, Mass Spectrometry

Copyright 2013 by the AAFS. Unless stated otherwise, noncommercial *photocopying* of editorial published in this periodical is permitted by AAFS. Permission to reprint, publish, or otherwise reproduce such material in any form other than photocopying must be obtained by AAFS. ** Presenting Author*