B88 Evaluation of the Analysis of Diamondoid Compounds in Kerosene Residues by Gas Chromatography/Mass Spectrometry for Use in Fire Debris Analysis

Heather Wert, and Thomas A. Brettell, PhD, Cedar Crest College, Department of Chemical & Physical Sciences, 100 College Drive, Allentown, PA 18104; and Vincent J. Desiderio, MS*

After attending this presentation, attendees will be able to better understand the gas chromatographic analysis of fire debris for diamondoid compounds, including adamantanes and diamantanes.

This presentation will impact the forensic science community by serving as new information and as a possible additional method in detecting kerosene residues in fire debris from suspicious fires.

Arson investigation has presented many problems for forensic scientists. For an investigation to be successful, being able to identify the accelerant and where it came from is of extreme importance. It has now been found that diamondoid compounds can be found in oil distillates of low or medium molecular weight, such as diesel or jets fuels, which can be used to determine a specific ion pattern for the fuel. This study will present an evaluation of the possible use of these diamondoid compounds for use in the analysis of fire debris samples, specifically where kerosene and other heavier fuels have been used.

Diamondoids are rigid, three dimensionally fused cyclohexyl alkanes which are naturally found in oil. The diamondoids can have anywhere from one cage (adamantane) to seven cages (heptamantane). The compounds may also have various functional groups attached increasing their molecular weight. The types of diamondoids and the ratio of the compounds found in a particular sample of oil have been found to be specific to the region of origin. These diamondoids have a high thermal stability and the heavy compounds are not easily affected by weathering or biodegradation which make them ideal for fire debris analysis. They are also conserved and concentrated during oil refining, creating a good internal standard. By using a combination of gas chromatography and mass spectrometry (GC/MS), a molecular ion fingerprint for the diamondoid component may be used to identify these fuels in fire debris. One microliter of carbon disulfide extract, or one milliliter of headspace, was injected into the gas chromatograph/mass spectrometer and a predetermined method ran with selected mass ions for particular diamondoid compounds. On the basis of GC/MS analysis, the principal diamondoids can be detected and monitoring in fire debris samples. Adamantanes were successfully isolated from liquid kerosene and adamantanes and diamantanes were isolated out of the headspace of kerosene samples. The diamondoids were confirmed through certified standards by GC/MS.

Currently most laboratories conducting fire debris analysis of fire debris samples use GC/MS, and have incorporated into their compilation of methods The American Society for Testing Materials (ASTM) standard methods (ASTM E-1618-06, June 1, 2006). The GC/MS method utilizes mass chromatography, the most widely used approach for the identification of flammable liquids in fire debris. This method is based on a chromatogram created from a series of ions in the mass spectrum which indicate the presence of a particular product. Monitoring the diamondoids could add another set of mass ion standards to search for, adding increased specificity to then identification. Since diamondoids are relatively heavy compounds and resist evaporation, they are ideal to search for in an evaporated sample. The fact that the types and amount of diamondoids found vary according to region or origin may also provide a way to distinguish the origin and possibly the brand of accelerant. This information could provide important investigative leads in arson investigations.

Fire Debris, Diamondoids, Adamantane

 ** Presenting Author*