A144 The Detection of Diamondoid Compounds in Ignitable Liquid Residues by Gas Chromatography/Mass Spectrometry, Part II

Heather Wert, BS, 1131 Alpha Avenue, Lebanon, PA 17046; Thomas A. Brettell, PhD, Cedar Crest College, Department of Chemical & Physical Sciences, 100 College Drive, Allentown, PA 18104; Vincent J. Desiderio, MS, New Jersey State Police, Central Laboratory, 1200 Negron Road, Hamilton, NJ 08691; and Nicholas D.K. Petraco, MS, John Jay College of Criminal Justice, Department of Science, 899 10th Avenue, New York, NY 10019*

After attending this presentation, attendees will understand the importance of analyzing diamondoid compounds found in various ignitable liquid residues.

This presentation will impact the forensic community by adding compounds to analyze in ignitable liquid residues. These compounds will increase specificity for petroleum distillates and be an aid as a possible source identification.

Various different types of petroleum products have been detected and identified during the analysis of debris recovered from suspicious fires. Due to the complex nature of the crude oil they are derived from and the various different refining processes they are subjected to, it should be no surprise that these products contain a rich assortment of organic compounds that are useful for their classification.

For the purpose of fire debris analysis, five major classes of organic compounds have been previously identified and routinely utilized to detect and classify the types of petroleum products that may be found. These compounds include: (1) Normal alkanes, (2) Aromatics, (3) Cycloalkanes/naphthenes, (4) Branched alkanes/isoparaffins, and (5) Indanes. Products encountered may differ in their content of compounds (e.g., normal alkanes predominate in distillates as opposed to aromatics in gasoline) or their ranges (e.g., light products contain more volatile components).

Recently, another class of organic compounds called diamondoids has been extensively studied in the environmental field for use in determining the origin of oil spills. These compounds consist of rigid, three-dimensionally fused cyclohexyl alkanes. They are naturally found in crude oils where they are formed from organic matter that decomposes around the oil. The production of diamondoid compounds via such means results in variable production in different crude stocks. These compounds are conserved during oil refining and, in some circumstances will become concentrated in final products. They are rugged compounds that resist both weathering and bio-degradation. Although they do have some industrial uses, they are rarely encountered outside of petroleum products making them very specific for the detection of and identification of such products.

Due to their rugged nature and specificity in petroleum products the addition of this class of compounds to analytical schemes in fire debris analysis would be of obvious importance. To this end, previous research by this group has found that diamondoids, specifically adamantanes, can be found in kerosene via both liquid and passive headspace sampling.[1]

This purpose of the current work was to investigate the feasibility of extending the range of products from kerosene to include light, medium, and additional heavy petroleum products, including both distillates and specialty products. For the purpose of detecting and identifying the compounds of interest gas chromatography/mass spectrometry (GC/MS) was performed on a range of products. Adamantane ions were successfully extracted from chromatograms obtained from samples prepared from both liquid dilutions and passive headspace extractions. Current research shows that the adamantanes can also be found in light, medium, and heavy petroleum distillates as well as naphthenic paraffinic products. The diamondoids that are detected produce an easily recognizable pattern across all of the types of petroleum-based products.

Upon examination of the diamondoid profiles in different products of the same class, peak area ratios were qualitatively observed to differ. In order to determine if these differences could be utilized for differentiation purposes, each sample was run multiple times (using both liquid dilution and passive headspace extraction), peak area ratios were calculated for all samples analyzed, and the resulting data were plotted in a three-dimensional scatter plot. Using these data, it was found that petroleum products from the same class could be differentiated from one another. These results suggest that adamantanes can be used as a tool to differentiate petroleum products.

Reference:

[1] Wert H, Brettell T, Desiderio, V. Evaluation of the Analysis of Diamondoid Compounds *in Kerosene Residues by Gas Chromatography/Mass Spectrometry for Use in Fire Debris Analysis*. Proceedings of the 60th Anniversary Meeting of the American Academy of Forensic Sciences, Washington DC, 2008, Abstract **#B88**.

Arson, Fire Debris, Diamondoids

 ** Presenting Author*