A207 The Investigation of Adamantanes in Various Petroleum Distillates

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After attending this presentation, attendees will be familiar with the results of the examination of adamantanes in petroleum distillates for the potential use in fire debris analysis by GC/MS.

This presentation will impact the forensic science community by describing a gas chromatographic-mass spectrometric method that could potentially add to the ASTM standard test method for ignitable liquid residues in extracts from fire debris samples. The addition of a new class of compounds, adamantanes, to the standard test method may lead to greater differentiation between petroleum products found at arson scenes.

In suspicious fires where a petroleum distillate has been used as an accelerant, it may become difficult to identify said petroleum distillate because of matrix and pyrolysis products. This type of analysis is challenging in that the matrix and/or pyrolysis products may contain compounds that co-elute or produce similar chromatographic patterns. It has been proposed that using diamondoids, specifically adamantanes, may aid in the ability to differentiate the distillates. Adamantane is a molecule consisting of three fused cyclohexane rings in chair formations. The cage structure of this molecule adds to its stability with a boiling point of 269˚C.

A number of petroleum distillates with varying amounts of weathering were examined using GC/MS for the presence of eleven (11) adamantanes with different functional groups: adamantane, 1-methyladamantane, 1,3-dimethyladamantane, 1,3,5-trimethyladamantane, 2-mehtyladamantane, cis-1,4-dimethyladamantane, trans-1,4- dimethyladamantane, 1,2-dimethyladamantane, 1-ethyladamantane, 1-ethyl-3-methyladamantane, and 2-ethyladamantane. Extracted ion profiles (EIPs) of the standard adamantanes were utilized for comparisons to the EIPs of various petroleum distillates including gasoline, diesel #2, kerosene, mineral spirits and jet fuel A. Mass to charge (m/z) ratios specific for the adamantanes (136, 135, 149, 150, 163, and 107), were used to screen various different petroleum products from all three ASTM classes of accelerants (light, medium and heavy petroleum distillates). All samples were analyzed as liquids (diluted with pentane as needed), static headspace (SHS) samples, and passive headspace (PHS) extracts using carbon disulfide as the extracting solvent.

It was determined that at least one adamantane was found in all samples except 50% weathered and 75% weathered diesel fuel. Gasoline samples, consisting of unweathered, 25%, 50%, 75% and 99% weathered samples, showed inconsistent results across three trials. They also showed the most "interference" from non-adamantane ions in the EIP. Diesel fuel, kerosene, and mineral spirits showed peaks consistent with those found in the EIP of the adamantane standards. The mineral spirits sample was allowed to weather to 25% and 50%. Again, these consumer samples showed peaks consistent with the adamantane standards. The mineral spirits samples proved to be the most consistent across the three trials showing the least amount of interference ion peaks from non- adamantane ions.

Seven other consumer products found on the ASTM E1618-06 table of flammable liquids, four of which were non-petroleum products, were purchased. Static headspace analysis was performed on these samples and it was determined that only the products made from petroleum distillates showed the adamantane ion peaks on the EIP. Samples that were not made from petroleum products had no adamantane ion peaks present.

Using this information, it is believed that the ASTM E1618-06 standard for fire debris analysis could be amended to include the ions for adamantane. With this amendment, it may be possible to improve the identification of petroleum distillates found in fire debris using ASTM E1618-06.

Petroleum Distillates, Adamantane, GC/MS

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