B177 The Benefits of High-Resolution Mass Spectrometry for the Identification of Ignitable Liquids

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Learning Overview: After attending this presentation, attendees will see that through the use of high-resolution mass spectrometry, ignitable liquids may be more readily identified as well as the estimation of the degree of weathering (or loss) as compared to traditional methodologies employing nominal-mass mass spectrometry.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by providing forensic scientists with a more precise method of identifying specific ignitable liquids.

The current method used to identify ignitable liquids consists primarily of pattern matching either the gas chromatogram or extracted-mass chromatograms of the unknown sample to the gas chromatogram or extracted-mass chromatograms of a reference sample. This is performed by computer software in conjunction with the analyst and is subject to possible bias, which may impact the results. The samples are also likely to undergo significant degradation and experience interferences due to evaporation, microorganism activity, matrix effects, or from the actual combustion. The potential degradation and interferences can remove or add compounds, which may further impact the identification ability. These missing or additional compounds can negatively impact the ability to properly match the obtained pattern to that of the reference sample.

Additionally, when comparing the mass spectra between the unknown and reference samples using common analytical approaches, only nominal mass (integer mass) is observed. Fractional mass differences can be utilized to correctly distinguish between the fragments in a sample, which in turn can be used to better identify the compounds in the questioned ignitable liquid. These identified compounds can then be used to classify the ignitable liquids by American Society for Testing and Materials (ASTM) standard practices. Having a method that can identify specific compounds gives more validity to identifying ignitable liquid samples than the standard pattern-matching practices. A quantitative element is gained, and the possibility of bias and misidentification by the analyst is reduced. The goal of this project is to demonstrate that high-resolution mass spectrometry can be used to better identify ignitable liquids based upon fragments fractional-mass values.

Known ignitable liquid samples were analyzed using a LECO® Pegasus® GC-HRT$^+$ 4D High Resolution Time-Of-Flight/Mass Spectrometry (TOF/MS). Reference samples were used to construct an accurate-mass library. The data collected underwent statistical analysis in order to group together relevant fragments that could be useful in identification. Then, the statistical data along with the library were used to identify unknown ignitable liquid samples. These unknown samples included both neat and weathered samples. Preliminary results showed that this technique would prove useful in the identification of ignitable liquids.

Ignitable Liquids, High-Resolution Mass Spectrometry, Gas Chromatography