A157 Compound-Specific Carbon and Hydrogen Isotope Ratios of Paraffin for Forensic Investigations

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After attending this presentation, attendees will appreciate the forensic isotopic information contained in paraffin and hydrocarbon component mixtures.

This presentation will impact the forensic science community by providing additional discriminating isotopic tools for in-depth paraffin and hydrocarbon investigations.

Paraffins and, in general, hydrocarbon mixtures have a high significance in forensic investigations. Paraffin products are used (e.g., for candles), to impregnate matches or in cosmetics. Hydrocarbons in general are also used as arson accelerants. Remnants of liquid products such as paraffin, petrol, or diesel can often be identified at the crime scene and sometimes on ignition devices, for example, safety matches or candles.

Presently, paraffins and other (volatile) hydrocarbon mixtures are mostly characterized using GC or GC/MS methods. Some successful research has also been done on characterization of paraffin-containing candle waxes as part of an extended arson investigation.[1]

Further discrimination can; however, be obtained by using ^{13}C and ^{2}H isotope information for each single paraffin or hydrocarbon component in the mixture. This will provide a whole new dimension to the characterization of these materials. A GC-IRMS/MS method was developed and validated. Validation results will be shown. The GC-IRMS/MS method was then applied to characterize candle waxes, paraffin products as used to impregnate safety matches, as well as hydrocarbon mixtures as used for lamp oils.

The additional discrimination of GC-IRMS/MS over the already strong discrimination provided by EA-IRMS will be demonstrated for candle waxes from candles of various brands and shops from the Netherlands that were previously investigated using gas chromatography in combination with bulk carbon and hydrogen isotope ratios.

For the second application, paraffin was extracted from wooden safety matches in the NFI collection of wooden safety matches with burnt and un-burnt samples. Initial compound-specific n-alkane ^{13}C and ^{2}H isotope data from 14 wooden sticks of six different brands of safety matches indicate a wide variation in isotope values from -10‰ to -80‰ VSMOW for hydrogen and -29‰ to -35‰ PDB for carbon. In addition, the effect of burning on the isotope ratios is shown to be negligible for these samples. Further statistical data evaluation using the technique of cluster analysis will be performed to evaluate the potential level of discrimination such as between and within packages of safety matches from one brand.

For the last GC-IRMS/MS application, nine lamp oils from the NFI lamp oils collection were used, nominally representing five different brands. Both for ^{13}C as well as for ^{2}H isotopes, a wide variation is observed. Single brand lamp oils as bought in various shops could easily be discriminated in this way.

The above investigations are only a first step in applying GC-IRMS/MS to hydrocarbon mixtures in a forensic context. For some applications (candles, cosmetics), method application appears to be straightforward. For other applications, further investigations will be required. For example, in arson investigations, remnants of hydrocarbon mixtures as used for accelerants will normally be strongly evaporated, skewing the isotope ratios of the components. Furthermore, pyrolysis products from other materials may be present in a fire residue sample, potentially resulting in complex chromatograms where the hydrocarbon components to be investigated cannot be separated from other components.

Reference:

1. Dogger J, van Breukelen M, Hendrikse JN, Schrader MA, van Grol M, van der Peijl GJQ. Discrimination of candle wax materials by gas chromatography (GC) and isotope ratio mass spectrometry (IRMS). *Proceedings of the American Academy of Forensic Sciences*, 61st Annual Meeting, Denver, February 17-21, 2009, 103-104.

GC-IRMS, Paraffin, Isotope

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