

TECHNICAL NOTE

Michael W. Gilbert,¹ B.S.

The Use of Individual Extracted Ion Profiles Versus Summed Extracted Ion Profiles in Fire Debris Analysis

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ABSTRACT: Mass spectrometry has become commonplace in the area of forensic fire debris analysis. The use of extracted ion chromatography can assist the fire debris analyst in distinguishing an ignitable liquid from interference due to pyrolysis or other contaminants. Often the individual extracted ion chromatograms are added together to give a profile of a specific class of compounds. Occasionally, the summed ion profile is still too complex to allow the identification of an ignitable liquid. In these instances, the individual ion profiles can be of better use. An example of the use of individual ion profiles versus summed ion profiles to identify an ignitable liquid in an actual case is presented.

KEYWORDS: forensic science, arson, fire debris, mass spectrometry

In recent years, the use of mass spectrometry in fire debris analysis has gained wide spread acceptance. Mass spectrometry allows the analyst to use extracted ion profiles to filter out interference from pyrolysis products or other contaminants that may make the identification of an ignitable liquid difficult. In extracted ion profiling, ions that are indicative for certain classes of compounds are sorted out and their intensities plotted versus time. Often, several ions for a class of compounds are extracted, and their extracted ion chromatograms (EIC) summed to give a profile for that class (1). The ASTM Standard Guide for Ignitable Liquid Residues in Extracts from Fire Debris Samples by Gas Chromatography-Mass Spectrometry (E 1618-94) provides a list of the ions that can be sorted for different classes of compounds of interest to the fire debris analyst. For example, ions 43, 57, 71, and 85 are extracted and summed to produce the aliphatic profile. In many cases, the summed extracted ion profiles allow for the easy identification of an ignitable liquid. In some instances, however, the sample can contain other compounds that are independent of the ignitable liquid, but that also contain significant levels of the ions of interest. When the individual ion profiles are added together, the resulting profile can still contain a high level of interference due to pyrolysis products. When this occurs, it can often be beneficial to the analyst to observe the individual extracted ion profiles. By further filtering out the interference, the individual profiles can help facilitate the identification of an ignitable liquid.

¹ Forensic chemist, Pinellas County Forensic Laboratory, Largo, FL. Received 17 June 1997; and in revised form 30 Sept. 1997 and 5 Dec. 1997; accepted 5 Dec. 1997.

Materials and Methods

Instrumental Conditions

All samples were run on a Hewlett-Packard (Palo Alto, CA) 5890A gas chromatograph coupled to a 5970 mass selective detector. One- μ L injections were made utilizing a HP 7673A autosampler. The column was a 30 m Rtx-1 (100% dimethyl polysiloxane) column (Restek, Bellafonte, PA) with an internal diameter of 0.25 mm and a film thickness of 0.25 μ m. A flow rate of 0.68 mL/min at 60°C and a split ratio of 20:1 were used. The initial oven temperature was held at 50°C for 2.5 min. The temperature was then ramped to 300°C at a rate of 15°C/min. The final temperature was held for 5.83 min, resulting in a 25 min run. The mass spectrometer was operated in scan mode with a scan range from 10 to 400 m/z.

Sample Preparation

Four samples were received from the agency in sealed paint cans. Item 1 contained a white T-shirt; item 2 a black pair of pants; item 3 part of a partially burned white, down comforter; and item 4 white paper towels that had been used to soak up a puddle suspected of containing an ignitable liquid.

The samples were extracted for 16 h at 60°C using 21 mm \times 8 mm activated charcoal strips (Albrayco Labs, Portland, CT). The charcoal strips were eluted with 200 μ L of carbon disulfide.

Results and Discussion

Summed extracted ion profiles were created using the following ions:

Aliphatic	43, 57, 71, 85
Aromatic	91, 105, 119
Cycloparaffins and alkenes	55, 69, 83
Naphthalenes	128, 142, 156

Analysis of item 1 failed to reveal the presence of an identifiable ignitable liquid, and items 3 and 4 were easily identified as gasoline. The total ion chromatogram of item 2 contained too much interference to be of significant assistance. The summed ion profiles of item 2 (Fig. 1) indicated the presence of gasoline (Fig. 2). The apparent differences in the aliphatic profiles of the gasoline standard and item 2 are due to the large presence of aldehydes in item 2, the relatively low concentration of aliphatics compared with aromatics in gasolines (especially above C7), and the wide variation in the aliphatic content of different gasolines. A closer examination of the aliphatic content of item 2 revealed a pattern comparable to that of the standard and the presence of saturated branched alkanes. However, the aromatic profile for item 2 con-

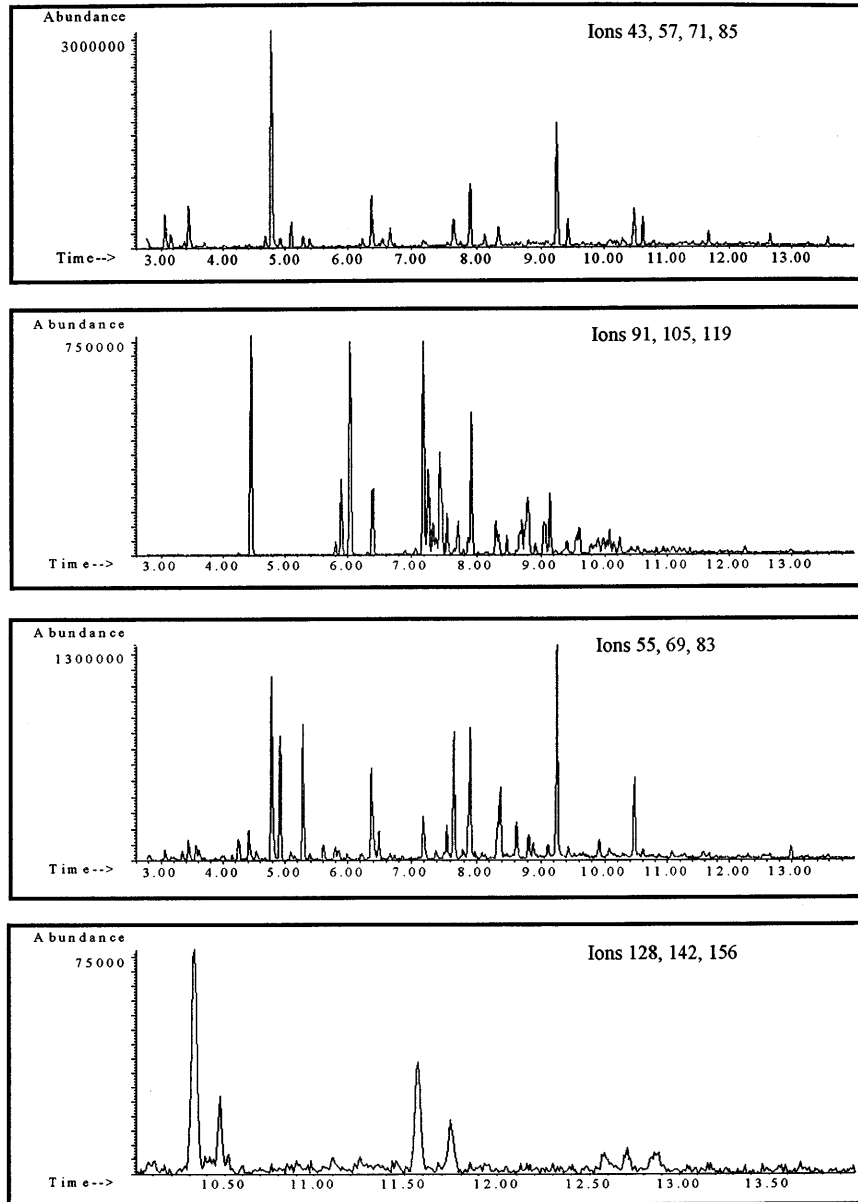


FIG. 1—Summed extracted ion profiles of item 2.

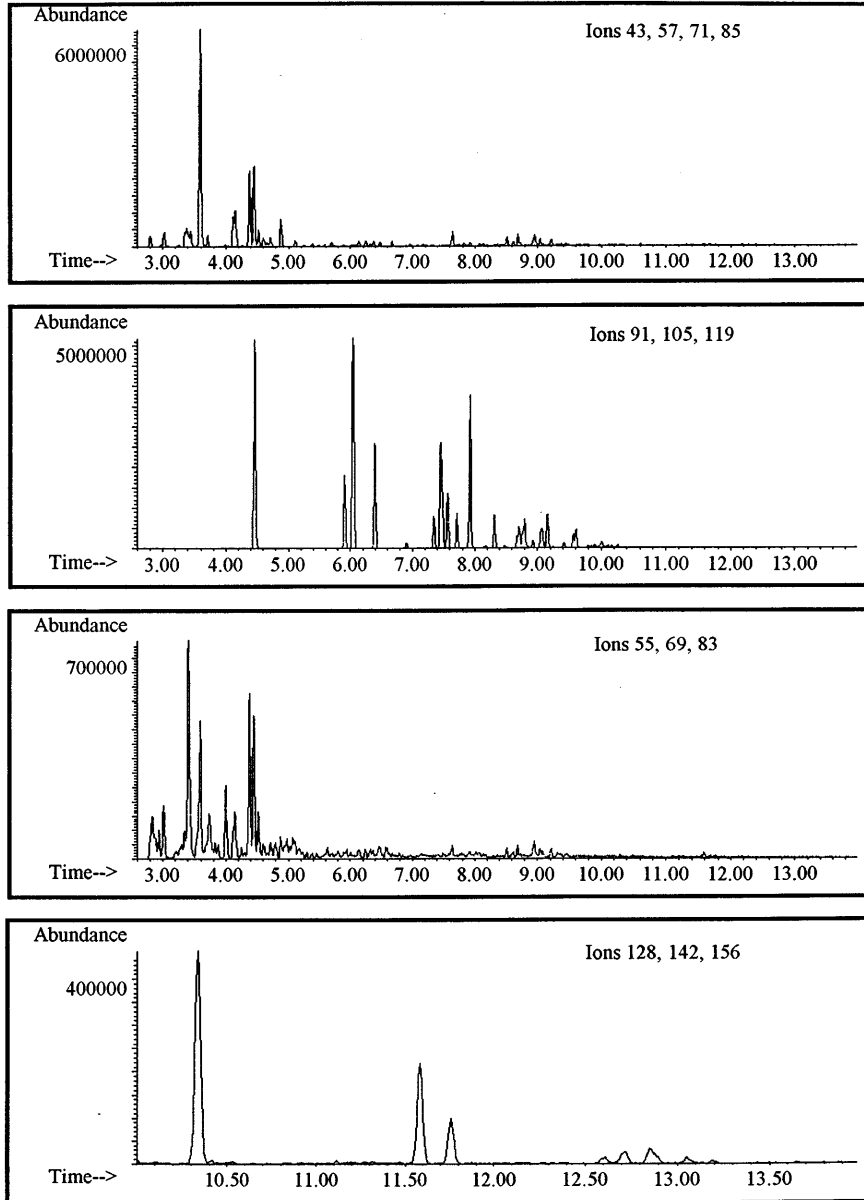


FIG. 2—Summed extracted ion profiles of gasoline.

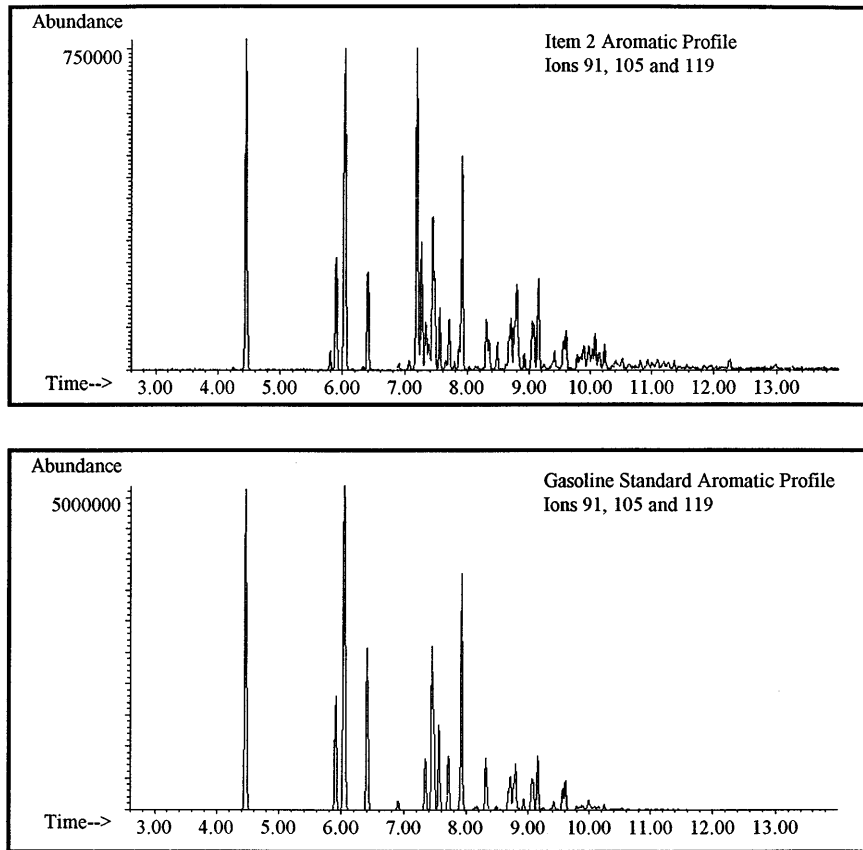


FIG. 3—Summed aromatic profiles (ions 91, 105, and 119) for item 2 (top) and gasoline standard (bottom).

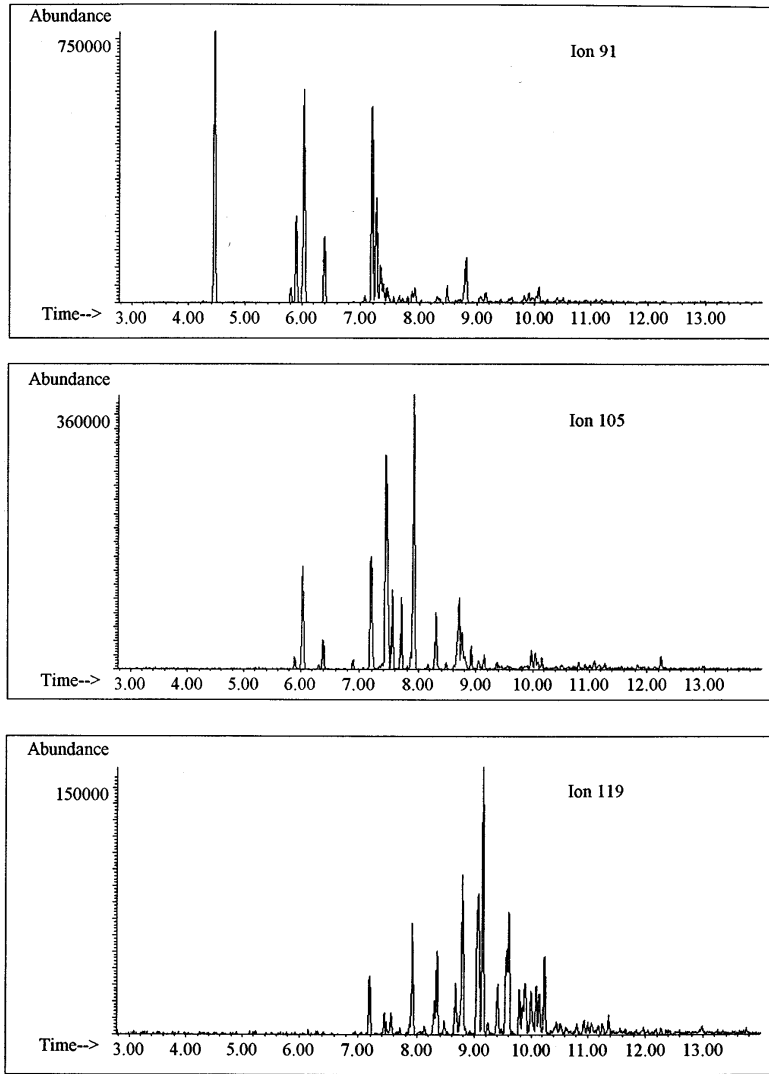


FIG. 4—Individual extracted ion profiles of item 2.

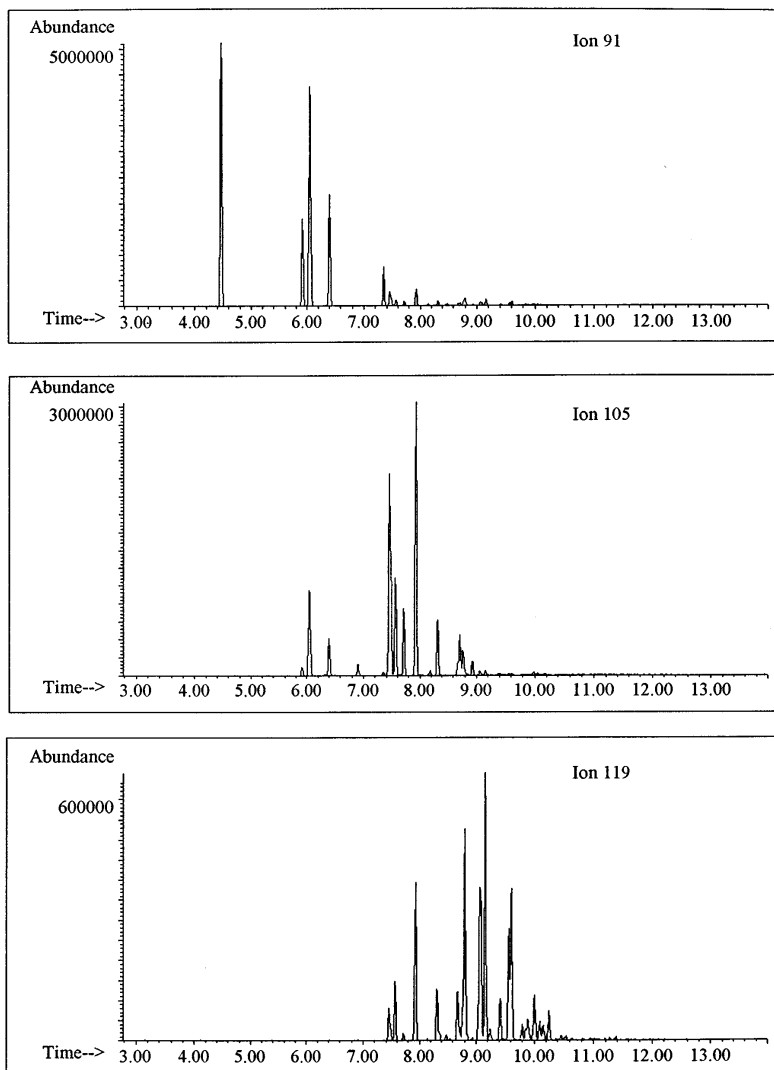


FIG. 5—Individual extracted ion profiles of gasoline.

tained extraneous peaks, most notably near the ethyltoluene group, which hindered the identification (Fig. 3). The compound that caused the greatest interference was identified as chlorotoluene.

Individual extracted ion chromatograms for item 2 (Fig. 4) and a gasoline standard (Fig. 5) were then obtained using ions 91, 105, and 119. Because the mass spectrum of chlorotoluene exhibits a base peak at m/z 91, it was observed in the EIC for ion 91. Ion 91 represents the toluene-ethylbenzene-xylene region in gasoline. This region of the pattern was affected by the presence of chlorotoluene, which eluted in the ethyltoluene range. Since the mass spectrum of chlorotoluene does not contain ions 105 and 119, it did not interfere with the identification using the extracted ion chromatograms for ions 105 and 119. Because the ethyltoluenes are dominated by a base peak at m/z 105, any interference by chlorotoluene was effectively removed, allowing for the easy identification of gasoline.

Conclusion

Mass spectrometry along with the use of extracted ion profiling can be a useful tool to the fire debris analyst. Profiles obtained by summed extracted ion chromatograms are often sufficient in

filtering interference to make an identification of an ignitable liquid. In many instances, however, interfering compounds which are not a part of the ignitable liquid are also extracted. These may be the result of pyrolysis or off-gassing by other materials in the sample. In these instances, individual extracted ion chromatograms may help to isolate any interfering compounds from the ignitable liquid, allowing for an identification of an ignitable liquid.

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Reference

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Additional information and reprint requests:
 Michael Gilbert
 Pinellas County Forensic Lab
 10850 Ulmerton Rd.
 Largo, FL 33778