R. Martin Smith.[1] *Ph.D.*

Mass Chromatographic Analysis of Arson Accelerants

ABSTRACT: We have developed a method for analyzing arson accelerants by computerized capillary gas chromatography mass spectrometry (GC/MS) in which the data produced is subjected to mass chromatography for sums of up to four ions at a time. Ions were chosen to represent major hydrocarbon families normally present in common arson accelerants and included m/z $57+71+85+99$ (aliphatics). $55+69+83+97$ (alicyclics and olefinics), $91+105+119+133$ (alkylbenzenes). $104+118+132+146$ (alkylstyrenes alkyldihydroindenes), $128+142+156+170$ (alkylnapthalenes). $178+192+206$ (alkylanthracenes). and $93+136$ (monoterpenes). Further mass chromatography for individual molecular ions often identified single components. Crude quantitative data were obtained from ion count measurements provided with the mass chromatograms by the data system. The range and pattern of aliphatic compounds, ratio of aliphatics to alicyclics (olefinics), relative concentrations of alkylbenzenes and alkylnaphthalenes, and presence or absence of unusual hydrocarbon families were found to distinguish between an assortment of standard accelerants and their evaporated residues.

KEYWORDS: chemical analysis, arson, accelerants

Gas chromatographic patterns of arson accelerants are often very characteristic, resulting in the almost universal use of this technique for the analysis of suspected arson residues [1,2]. However, recent reports of possible misinterpretation of gas chromatographic data from arson cases [3,4] prompted us to research the use of computerized gas chromatography/mass spectrometry (GC/MS) for more conclusive identification of the organic compounds present in these residues.

Previous reports of arson work using GC/MS were fairly limited in scope, dealing mainly with specific sample types [2,5] or with individual cases [3]. In fact our own prior work in this area was confined primarily to instances where only a few easily separable GC peaks were encountered [6]. The appearance of recent generation computerized GC/MS models, equipped for high speed collection and sophisticated manipulation of mass spectral data, has made this technique much more attractive for routine arson work than previously.

Experimental Procedures

Accelerants

Standard accelerants were obtained from local commercial outlets and were used without modification. Evaporated standards were generated simply by allowing the original liquids to evaporate at room temperature for periods ranging from several days up to twelve months.

GC/MS Analyses

Whenever possible, samples were injected by the wet needle technique, with injection sizes on the order of 0.1 μL. Samples that were too viscous or too small to inject by this method were dissolved in carbon disulfide and 0.5 to 1.0 μL of the resulting solutions were used. An exception was used for the evaporated low-boiling naphtha samples, where a small amount of original liquid was added to the highly evaporated residues, then allowed to approach dryness again. This produced small amounts of artificial contamination by the original liquids in chromatograms of these evaporated products.

Combined glass capillary GC/MS was performed on a Dupont DP-102 GC/MS equipped with a capillary injector and a Supelco 30-m SP-2100 WCOT column. The injector (200°) was used exclusively in the split mode (split ratio aproximately 55/1). A linear helium flow of about 33 cm/s was measured through the column, and helium makeup gas was added to the column effluent to provide a flow of about 25 mL/min through the glass jet separator at 250°.

A single temperature program accommodated most samples: the GC oven was held at 50 $\pm$ 2° for 8 min following injection, then the temperature was increased at 3.9°/min for 51.5 min to reach a final oven temperature of 250°. Although condensed polynuclear aromatic hydrocarbons much larger than alkylanthracenes were not detected using this program, the absence of such compounds did not seem to be critical for sample characterization.

The capillary system and temperature program were calibrated before each set of runs with a mixture of n-alkanes (C_5 to C_{16}, retention times—1.7 to 39.5 min) and on a daily basis with a set of C_5 to C_9 n-alkane standards. This system proved remarkably stable even after repeated exchanges of the capillary column with a packed column used routinely for drug analysis.

The electron impact mode (75 eV) was used exclusively for mass spectrometry with a source temperature of 175 to 200°. Spectra were collected at a scan rate of 128 AMU/s over a range from m/z 35 to 250. Compounds with higher molecular weights rarely were indicated in these samples under the GC conditions used.

Mass Chromatographic Method

GC/MS analysis of arson samples was not as straightforward as we thought at first. During our first encounters with many samples, we tried to identify each peak in the obviously complex chromatograms using a computer search of the 35 000 spectrum National Bureau of Standards library. Overall, however, this approach was not productive. Despite the large number of components separated by these chromatographic conditions, many GC peaks remained unresolved mixtures of two, and often more, components. Individual compound identification under these circumstances was difficult at best, and virtually impossible for many compounds [7]. Also, the library search task itself was laborious, requiring about 3 to 4 h to work through samples of this complexity. More discouraging, even those peaks that appeared to be chromatographically pure often gave ambiguous library search results. For example, many of the molecular weight 120 alkylbenzenes were all identified as 1, 2, 3-trimethylbenzene, while several others were identified as the 1, 2, 4-isomer. Clearly without a library of standard spectra run on our instrument for all of the individual components, this method could have only limited success.

We hoped to improve individual component analysis of the samples using mass chromatography, a technique in which the computer searches through each mass spectrum obtained in a sample run for the presence of selected ions (or a sum thereof) and plots out a chromatogram corresponding only to the relative concentrations of these ions [8]. Theoretically, chromatograms showing only compounds having specified molecular weights or fragmentation patterns (our data system allowed us to look for sums of up to four ions at a time) would help us locate individual components more easily and perhaps enhance the quality of the individual mass spectra [9]. A careful study of mass spectra generated during

early runs of standard accelerants and consultation with standard texts [10] indicated that only a few types of spectra accounted for a vast majority of all of the compounds present:

1. Saturated aliphatic hydrocarbons (straight chain and branched). These were best characterized by major fragment ions at m/z 57, 71, 85, and 99, and to a much lesser extent by the individual molecular ions at m/z 100, 114, 128, and so forth.

2. Alicyclic and unsaturated aliphatic (olefinic) hydrocarbons. Both exhibited large fragment ions at m/z 55, 69, 83, and 97.

3. Alkylbenzenes. These compounds showed intense fragment ions at m/z 91, 105, 119, and 133, as well as giving substantial molecular ions at m/z 92, 106, 120, and so forth.

4. Alkyl-substituted condensed polynuclear aromatics. Most exhibited intense molecular ions, such as methylnaphthalene (m/z 142), anthracene (m/z 178), and so forth.

Other groups of compounds occurring less frequently included monoterpenes ($C_{10}H_{16}$), characterized by the molecular ion (m/z 136) and by a large fragment ion at m/z 93; alkyl-styrenes and the isomeric dihydroindenes and tetrahydronaphthalenes, all with intense molecular ions at m/z 104, 118, 132, and 146; and alkylbiphenyls and isomeric acenaphthenes at m/z 154, 168, 182, and so forth.

A mass chromatogram corresponding to each family of compounds was calculated by summing the intensities of up to four ions characteristic of that group (thus, the mass chromatogram for saturated aliphatic hydrocarbons was calculated by adding the intensities of the m/z 57, 71, 85, and 99 ions from each mass spectrum in the sample run). The results, accomplished in about 5 min of computer time for a typical 40- to 60-min capillary GC run are illustrated in Fig. 1 for evaporated gasoline. This technique improved our library search results somewhat, but more significantly it emphasized to us the wealth of highly specific information contained in the mass chromatograms themselves.

The mass chromatograms corresponding to "NAPHTHALENES" and "POLYNUCLEAR AROMATICS" in the evaporated gasoline sample (Fig. 1, Chromatograms 6 and 8) illustrate this most clearly. Both chromatograms strongly suggest a homologous series of compounds in which the number of structural possibilities for each member increases after starting from a structurally unique lowest member. Recalling that the mass spectra of higher boiling aromatic compounds were characterized by intense molecular ions, we found that, by calculating individual mass chromatograms for each molecular ion as well as for the sum, each cluster of peaks in the summed chromatogram corresponded to a set of isomeric compounds (confirmed by visual examination of the individual spectra and by library search). Figures 2 and 3 show this for the alkylnaphthalene and alkylanthracene series in evaporated gasoline. In Fig. 2 the structurally unique naphthalene gave a single GC peak, the methylnaphthalenes (two isomers possible) gave two peaks, the C_2-naphthalenes (twelve isomers possible) gave at least five peaks, and so forth. The extraneous peak in the m/z 170 chromatogram at $t = 24.8$ min is due to the molecular ion of n-dodecane.

Similar results for the alkylbenzenes of unevaporated gasoline are shown in Fig. 4. Note that individual components of significant intensity such as benzene and toluene have been extracted from an equally intense background of interfering peaks.

Although location and identification of individual aromatic compounds, or at least families of isomeric aromatics, by this method proved relatively easy, specific information about aliphatic and alicyclic compounds was more elusive. Mass chromatograms corresponding to these components usually gave no detectable patterns at all, although in some instances individual mass chromatograms of the n-alkane molecular ions and comparison of retention times to those of known standards confirmed the presence of these compounds as major constituents of samples such as fuel oil (Fig. 5).

Even though identification of many individual components of typical arson accelerants was thus greatly facilitated using mass chromatography, the identification of a possible accelerant in an actual arson residue did not necessarily follow, since many of these products
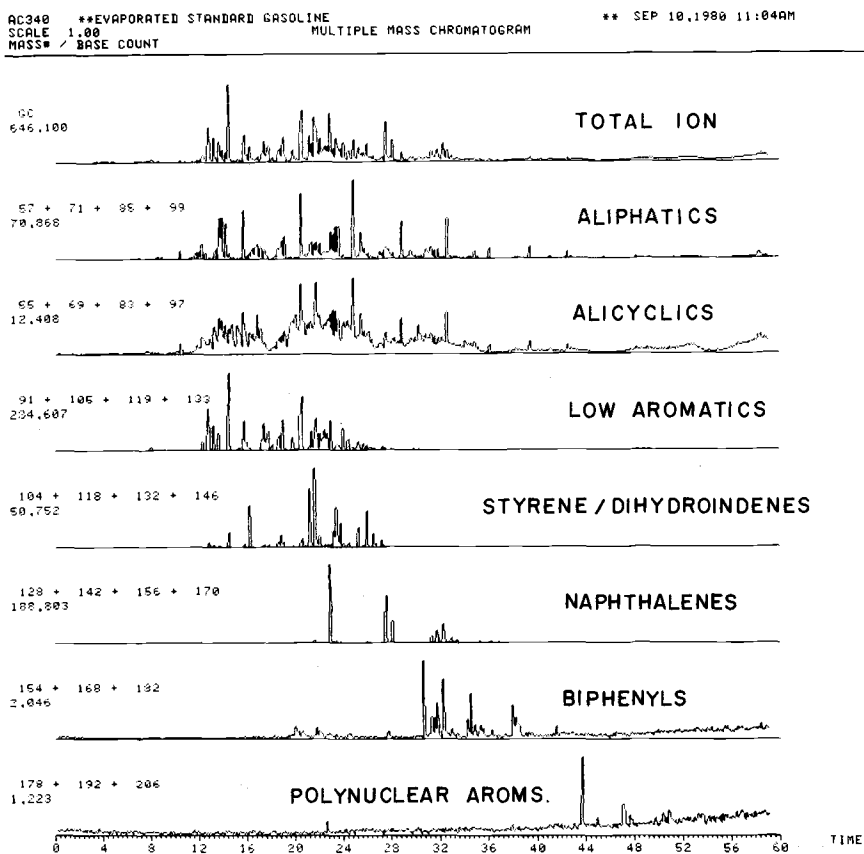
AC340   **EVAPORATED STANDARD GASOLINE   ** SEP 10,1980 11:04AM
SCALE 1.00   MULTIPLE MASS CHROMATOGRAM
MASS* / BASE COUNT

FIG. 1—*Mass chromatograms of hydrocarbon families in evaporated gasoline.*

are mixtures of essentially the same compound types which, by virtue of differences in manufactural processing [11] and collection of different distillation cuts [12], are found in these accelerants in varying proportions. Fortunately a very crude quantitative measure of the relative concentrations of many compounds was provided by the data system as the total ion count for the largest GC peak in each chromatogram (shown in small print at the left end of each chromatogram, see Figs. 1 to 5). These numbers cannot possibly give truly accurate concentrations since they do not account for such variables as fragmentation percentages. However, they still seemed to be useful indicators of relative proportions of the various compounds or compound types, especially since they were derived in the same manner for each sample.

Standard Accelerants

To evaluate whether we could adequately characterize typical accelerants by this method, we examined twelve common volatile hydrocarbon mixtures from different sources and several of their evaporated residues. Mass chromatographic data for these samples, consisting of ion counts for the compounds and compound types described above, are listed in Table 1. A careful study of these data showed that each family of compounds gave useful information for distinguishing between the different samples.
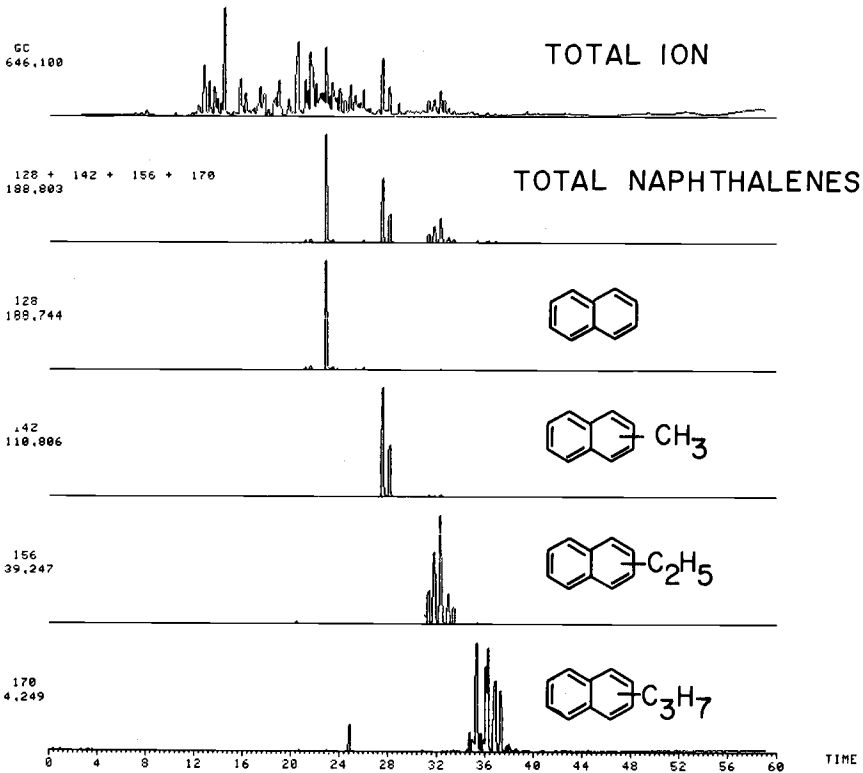
FIG. 2—*Mass chromatograms of alkylnaphthalenes in evaporated gasoline. Individual isomeric clusters were located using molecular ion chromatograms.*

Aliphatics

The pattern of aliphatic hydrocarbons was easily determined only when n-alkanes were present as a series of intense, nearly equidistant peaks (see Fig. 1, Chromatogram 2 and Fig.5). In other cases retention times of nearby compounds were compared with those of standard n-alkanes to help establish the general molecular weight range for the sample. When present, the identity of the n-alkanes was often confirmed by library search and always by comparison of retention times with those of known standards.

Many samples showed characteristic ranges of n-alkanes, which proved particularly useful for making distinctions among accelerant classes (for example, gasoline versus fuel oil or paint thinner versus low-boiling naphthas). It also differentiated between regular gasoline and aviation fuel, both of which contained unusually high concentrations of aromatic compounds. Several of the evaporated samples gave unusual patterns of aliphatic compounds, but the "bimodal" distribution of alkanes in the low-boiling naphtha samples reflected sampling procedures rather than realistic conditions (see Experimental Section). The low-boiling members of these series normally would have evaporated under the extreme temperatures of an actual fire.
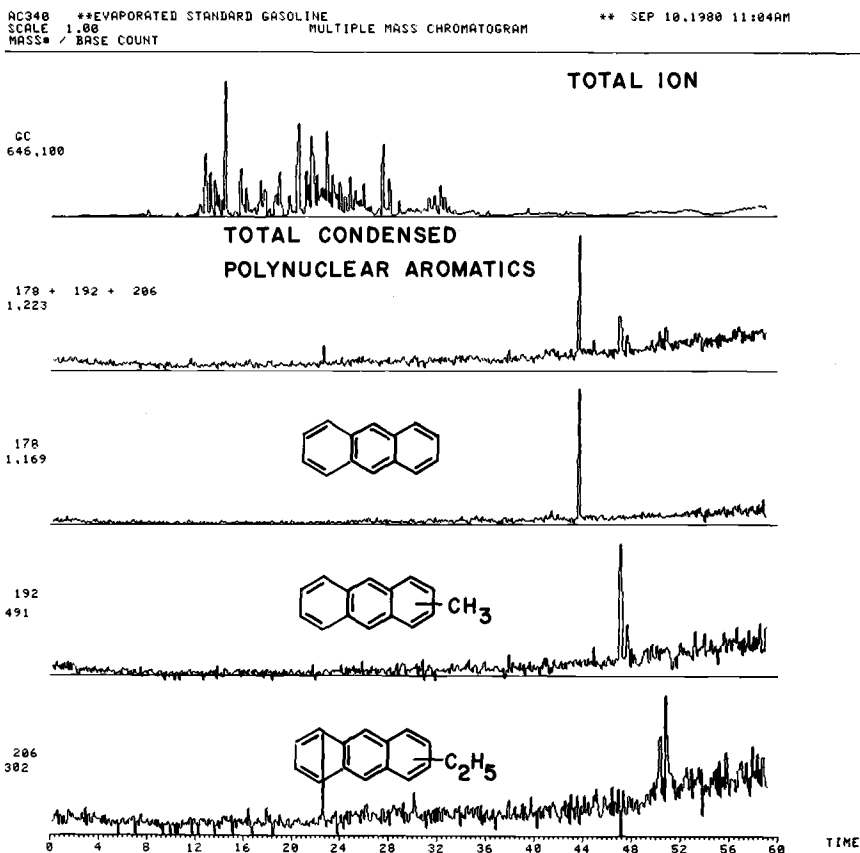
AC340   **EVAPORATED STANDARD GASOLINE   ** SEP 10,1980 11:04AM
SCALE 1.00   MULTIPLE MASS CHROMATOGRAM
MASS* / BASE COUNT

FIG. 3—*Mass chromatograms of alkylanthracenes in evaporated gasoline.*

Alicyclics

Individual compound identification for this group was often tedious and rarely productive. In some instances where low concentrations of alicyclics were indicated, the pattern for these compounds actually mimicked that of the aliphatics, reflecting the fragmentation of the latter compounds to give the m/z 55, 69, 83, and 97 series of ions, although in considerably smaller amounts. However, the ratio of aliphatic to alicyclic hydrocarbons was distinctive of several products. Both "Benzine" low-boiling naphtha and Coleman® fuel showed significantly higher concentrations of alicyclics than aliphatics, while paint thinners contained intermediate amounts of alicyclics and charcoal lighter fluid consisted almost entirely of aliphatics. Alicyclic compounds seemed much more prone to evaporation than either the aliphatics or any of the aromatics, as nearly all of the evaporated residues examined had lower relative proportions of alicyclics than did the original products.

Alkylbenzenes and Alkylnaphthalenes

Compounds in these groups were usually the easiest to identify and generally afforded good library search matches. The relative concentrations of alkylbenzenes were estimated best from individual molecular ion (Fig. 4), rather than family fragment ion, chromatograms
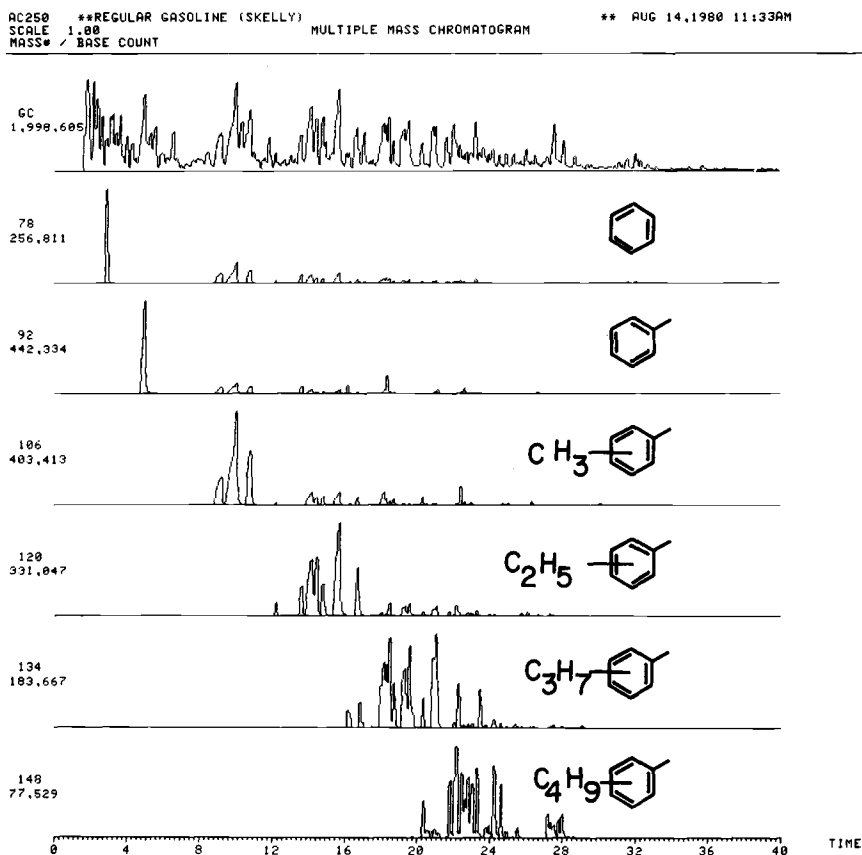
FIG. 4—*Molecular ion chromatograms of isomeric alkylbenzenes in regular gasoline.*

because of overlapping retention times between various isomeric groups. In addition, benzene (molecular weight 78) was missed entirely in the family chromatograms, while other compounds having different molecular weights often gave fragment ions at the same mass (for example, both toluene and the xylenes had large fragment ions at m/z 91).

One of the sharpest distinctions between many samples was the presence or absence of various aromatic compounds, especially the alkylbenzenes and alkylnaphthalenes. High percentages of these compounds were almost uniquely characteristic of evaporated gasoline (see also Ref 2). Although aviation fuel contained similar amounts of low-boiling alkyl-benzenes, it lacked significant quantities of higher-boiling alkybenzenes and alkylnaph-thalenes which were prominent in the evaporated gasoline total ion chromatogram. Other samples with boiling ranges similar to that of evaporated gasoline, such as fuel oil and diesel fuel, were noticeably more deficient in all of these aromatics. This single feature could help distinguish between evaporated gasoline and fuel oil, which might not always be possible by conventional GC.

Accelerants apparently devoid of aromatic hydrocarbons included charcoal lighter fluid, which retained this condition even upon evaporation, and the low-boiling naphthas. Extreme evaporation of the latter, however, revealed small but characteristic quantities of alkylnaphthalenes. Paint thinners, having significant concentrations of middle-boiling alkyl-benzenes but few alkylnaphthalenes, were between the extremes.
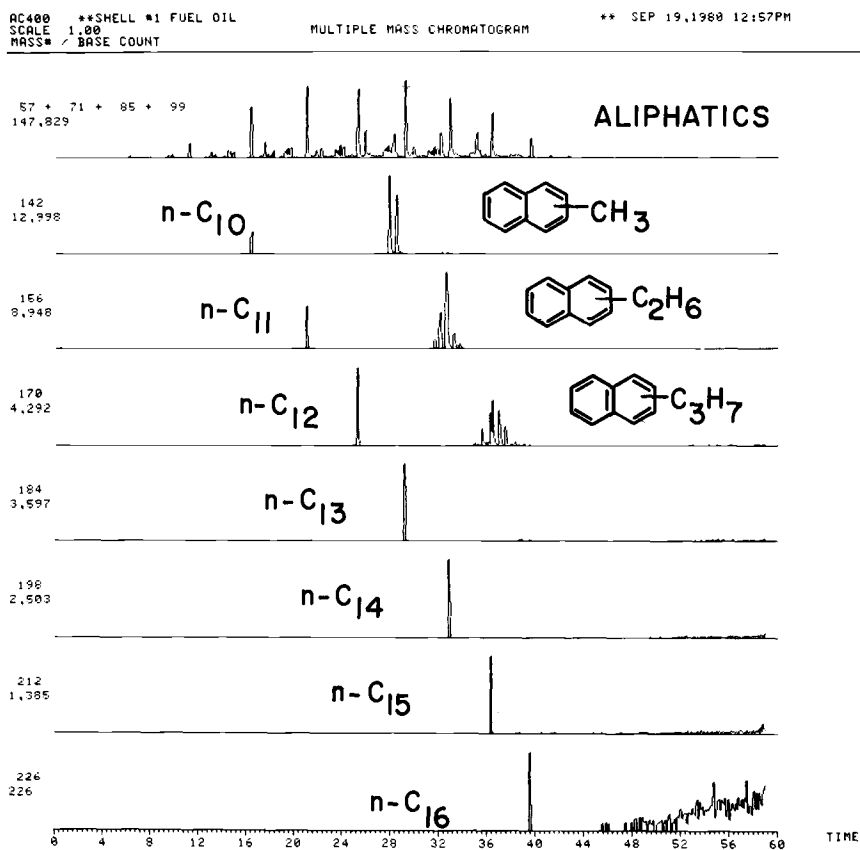
FIG. 5—*Fragment ion mass chromatogram of aliphatics and molecular ion chromatograms of individual n-alkanes in fuel oil. Alkylnaphthalene molecular ions occur at the same masses, but at longer retention times.*

High Aromatics

Alkylanthracenes or alkylphenanthrenes were not observed in any of the unevaporated samples, but were found upon evaporation of several products of moderate to high volatility—most notably gasoline, aviation fuel, and the low-boiling naphthas. Our failure to detect these compounds in high-boiling petroleum fractions such as fuel oil and diesel fuel may reflect only the resistance of these materials to appreciable evaporation under the relatively mild conditions used.

Terpenes

These compounds were conspicuously absent from accelerants derived from crude oil, but were highly characteristic of turpentine, a product in which virtually no other type of hydrocarbon was present. On the other hand, petroleum-based accelerants often gave weakly positive responses for this family, since alkylbenzenes with fragment ions at m/z 91 or molecular ions at m/z 134 sometimes gave isotope peaks large enough to produce peaks at m/z 93 and 136 on mass chromatography. In these cases, however, the "terpene" mass chromatographic pattern closely resembled that produced by the alkylbenzenes, rather than that of products

TABLE I. MASS CHROMATOGRAPHIC ANALYSIS OF STANDARD VOLATILES

SAMPLE	TOTAL ION COUNT[a]	ALIPHATICS 57+71+85+99	n-ALKANES PRESENT	n-ALKANES MAXIMUM	ALICYCLICS 55+69+83+97	LOW AROMATICS 91+105+119+133	BENZENE 78	TOLUENE 92	XYLENES 106	C_3-AROMATICS 120	C_4-AROMATICS 134
REGULAR GASOLINE	2000	490 (24.5)[b]	5-16+	10-11	320 (16.0)	700 (35.0)	256 (12.8)	442 (22.1)	403 (20.2)	331 (16.6)	184 (9.2)
FUEL OIL (#1)	331	148 (44.7)	8-17	11-13	25 (7.6)	23 (6.9)	--	1 (0.3)	5 (1.5)	23 (6.9)	14 (4.2)
DIESEL FUEL	6297	2272 (36.0)	9-20+	12-15	535 (8.5)	218 (3.5)	4 (.07)	28 (0.4)	53 (0.8)	137 (2.2)	87 (1.4)
AVIATION FUEL	6279	2011 (32.0)	5-9	5-6	N.A.[d]	1041 (16.6)	89 (1.4)	1040 (16.6)	600 (9.6)	400 (6.3)	200 (3.2)
GULF-LITE[TM] CHARCOAL LIGHTER	396	223 (56.3)	(8-16)[e]	---	19 (4.8)	N.P.	--	--	--	--	--
COLEMAN[TM] STOVE AND LANTERN FUEL	5457	1868 (34.3)	5-11	7-9	2048 (37.6)	336 (6.2)	80 (1.5)	176 (3.2)	189 (3.5)	41 (0.8)	7 (0.1)
DEODORINE PAINT THINNER	1805	697 (38.6)	8-12, 14,16	10-11	320 (17.7)	253 (14.0)		--	9 (0.5)	147 (8.1)	47 (2.6)
THINOLENE PAINT THINNER	551	229 (41.6)	8-13	10-11	126 (22.8)	91 (16.5)	.5 (.05)	4 (0.7)	7 (1.3)	52 (9.4)	21 (3.8)
BENZINE (Low-boiling Naphtha)	322	110 (34.2)	(7-9)[e]	---	129 (40.1)	1.4 (0.4)	--	.5 (0.2)	1.4 (0.4)	--	--
RONSONOL[TM] LIGHTER FLUID (Low-boiling Naphtha)	235	81 (34.5)	7-9	8	64 (27.2)	15.2 (6.5)	--	15.2 (6.5)	14.5 (6.2)	--	--
JON-E WARMER FLUID (Low-boiling Naphtha)	2516	816 (32.4)	7-9	8	218 (8.7)	110 (4.4)	--	76 (3.0)	63 (2.5)	--	--
MR. THINZIT[TM] TURPENTINE	2234	N.P.	---	---	N.P.	N.P.	--	-.-	--	--	--
EVAP. REGULAR GASOLINE	646	70 (10.8)	8-19	11-12	12 (1.9)	234 (36.2)	--	--	20 (3.1)	234 (36.2)	160 (24.8)
EVAP. AVIATION FUEL	981	500 (51.1)	9-10	9-10	33 (3.4)	123 (12.5)	--	--	--	56 (5.7)	52 (5.3)
EVAP. WIZARD[TM] CHARCOAL LIGHTER	249	97 (38.9)	12,14 16,18	14,16	20 (8.0)	N.P.	--	--	--	--	--
EVAP. COLEMAN[TM] FUEL[f]	6123	2784 (45.5)	10-12	10-11	1015 (16.6)	120 (2.0)	--	--	--	16 (0.3)	58 (0.9)
EVAP. DEODORINE PAINT THINNER	852	388 (45.5)	10-12	10-11	124 (14.5)	117 (13.7)	--	--	--	--	50 (5.9)
EVAP. BENZINE (Low-boiling Naphtha)	1149	393 (34.2)	(7-9)[e], 14-20+	16-18	305 (26.5)	N.P.	--	--	--	--	--
EVAP. RONSONOL[TM] (Low-boiling Naphtha)	4732	367 (7.8)	7-20+	13-14	254 (5.4)	413 (8.7)	--	--	--	N.A.	N.A.
EVAP. JON-E WARMER FLUID[f] (Low-boiling Naphtha)	1740	551 (31.7) 11-20	7-8,	16-17	163 (9.4)	63 (3.6)	--	.5 (.03)	1.1 (.06)	N.A.	N.A.

[a]All ion counts are given in thousands of ions.
[b]Numbers in parentheses show percentage of total ion count.
[c]N.P. - No pattern to indicate the presence of specific compounds.
[d]N.A. - Data not available for this compound or group.
[e]No n-alkanes observed; general range of branched alkanes shown.
[f]An important constituent of these samples was butylated hydroxytoluene (BHT), a common anti-oxidant (M.W. 220; ret. time about 36 min).

TABLE I. (Cont'd)

C_5-AROMATICS 148	TERPENES 93+136	NAPHTHALENE 128	Me-NAPHTHALENES 142	C_2-NAPHTHALENES 156	C_3-NAPHTHALENES 170	STYRENE 104	METHYLSTYRENES 118	C_2-STYRENES 132	C_3-STYRENES 146	ANTHRACENE 178	Me-ANTHRACENES 192	C_2-ANTHRACENES 206
77 (3.9)	N.P.[c]	311 (15.6)	311 (15.6)	100 (5.0)	5 (0.5)	25 (1.3)	171 (8.6)	130 (6.5)	70 (3.5)	--	--	--
8 (2.4)	N.P.	9 (2.7)	13 (3.9)	10 (3.0)	3 (0.9)	N.P.	N.P.	N.P.	N.P.	--	--	--
48 (0.8)	N.P.	131 (2.1)	498 (7.9)	480 (7.6)	170 (2.7)	N.P.	N.P.	40 (0.6)	153 (2.4)	--	--	--
--	N.P.	96 (1.5)	92 (1.2)	16 (0.3)	2 (.04)	54 (0.9)	19 (0.3)	11 (0.2)	3 (.07)	--	--	--
--	N.P.	--	--	--	--	--	--	--	--	--	--	--
--	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	--	--	--
11 (0.6)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	--	--	--
6 (1.1)	N.P.	11 (2.0)	3 (0.5)	--	--	N.P.	N.P.	N.P.	N.P.	--	--	--
--	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	--	--	--
--	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	--	--	--
--	647 (29.0)	--	--	--	--	N.P.	N.P.	N.P.	N.P.	--	--	--
80 (12.4)	N.P.	188 (29.1)	110 (17.0)	39 (6.0)	4 (0.7)	--	28 (4.3)	39 (6.0)	5 (0.8)	1.2 (0.2)	0.4 (.06)	0.2 (.03)
8 (0.8)	N.P.	143 (14.6)	130 (13.3)	50 (5.1)	10 (1.0)	--	5 (0.5)	17 (1.7)	6 (0.6)	7 (0.7)	4 (0.4)	1 (0.1)
--	N.A.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	--	--	--
30 (0.5)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.[g]	N.P.	N.P.	N.P.	--	--	--
117 (13.7)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	--	--	--
--	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	50 (4.4)	6 (0.5)	1.5 (0.1)
N.A.	850[h] (18.0)	20 (0.4)	33 (0.7)	40 (0.8)	12 (0.3)	N.P.	N.P.	N.P.	N.P.	23 (0.5)	5.5 (0.1)	2 (.04)
N.A.	N.P.	4 (0.2)	8 (0.4)	26 (1.5)	38 (2.2)	N.P.	N.P.	N.P.	N.P.	160 (9.2)	24 (1.4)	5 (0.3)

[g] A compound giving a large fragment ion at m/z 104 proved to be phenylcyclohexane.
[h] The major peak in the total ion chromatogram was an unidentified terpene alcohol; several aromatic esters, aldehydes, and sulfonamides were present also.

such as turpentine. We found that individual compound identification by library search was vital for establishing the actual presence of terpenes.

Surprisingly, one other standard, evaporated lighter fluid, showed significant amounts of terpenoid compounds (confirmed by library search). However, the compounds observed in this sample had very different retention times from those in turpentine and were identified as terpene alcohols (molecular weight 152).

Other Families

Other compounds seemed to have limited use in sample identification and also seemed most prone to produce confusing data. Careful identification of individual compounds in these groups by library search or retention time comparison or both was always warranted, since several spurious compounds were found to give fragment ions (or isotopes of fragment ions) which appeared in these families.

The relatively high concentrations of styrenes and dihydroindenes found in gasoline and aviation fuel were interesting, but merely confirmed conclusions drawn from the relative concentrations of other groups. On the other hand, styrene and related compounds were often abundant in many authentic arson residues [13], but in many instances were ascribable to the decomposition of styrene-containing polymers [3,14]. Several unusual compounds were discovered by individual spectrum analysis of unfamiliar mass chromatograms, but only the mixture of terpene alcohols, aromatic esters, aldehydes, and sulfonamides found in evaporated Ronsonol® seemed distinctive.

Conclusions

Semiquantitative mass chromatography adds an enormous amount of supportive information about the chemical makeup of an arson sample. Some of this information is undoubtedly available from other sources, such as comparison of GC retention times or a spectrum-by-spectrum analysis of a GC/MS run. These methods tend either to be tedious or less informative, and in neither case can they combine relatively specific individual compound identification with at least crude quantitation, both of which are desirable for accelerant identification. Gas chromatography alone certainly can be used to identify arson accelerants, but we have found many GC patterns that do not match any known standards or, even worse, patterns that nearly match those of standards but are not quite convincing. Chemical information about the compounds present in those samples would be most helpful. We believe that the rapidity and informational value of this method makes it extremely useful for differentiating among the various arson accelerants. Our researches into applications of this method to actual arson residues continue.

References

[1] Camp, M. J., "Analytical Techniques in Arson Investigation," *Analytical Chemistry*, Vol. 52, No. 3, March 1980, p. 422A–426A.

[2] Mach M. A., "Gas Chromatography-Mass Spectrometry of a Simulated Arson Residue Using Gasoline as an Accelerant," *Journal of Forensic Sciences*, Vol. 22, No. 2, April 1977, pp. 348–357.

[3] Juhala, J. A., "Determination of Fire Debris Vapors Using an Acid Stripping Procedure with Subsequent Gas Chromatography and Gas Chromatography/Mass Spectrometry," *Arson Analysis Newsletter*, Vol. 3, No. 4, Oct. 1979, pp. 1–19.

[4] Emmermann, L., "Arson 'Expert' Admits That He Lied Under Oath," *Chicago Tribune*, Vol. 133, No. 153, 1 June 1980, pp. 1, 8.

[5] Mauceri, L. A. and Bowden, J. P., "Selection of Residue and Vapors From a Simulated Drug Lab Fire," *Arson Analysis Newsletter*, Vol. 4, No. 2, Oct. 1980, pp. 1-10.

[6] Smith, R. M., "Some Applications of GC/MS in the Forensic Laboratory," *American Laboratory*, Vol. 10, No. 5, May 1978, pp. 53-60.

[7] Rosenthal, D., "Theoretical Limitations of Gas Chromatographic/Mass Spectrometric Identification of Multicomponent Mixtures," *Analytical Chemistry*, Vol. 54, No. 1, Jan. 1982, pp. 63-66.

[8] Hites, R. A. and Biemann, K., "Computer Evaluation of Continuously Scanned Mass Spectra of Gas Chromatographic Effluents," *Analytical Chemistry*, Vol. 42, No. 8, July 1970, pp. 855-860.

[9] Biller, J. E. and Biemann, K., "Reconstructed Mass Spectra, A Novel Approach For the Utilization of Gas Chromatograph/Mass Spectrometer Data," *Analytical Letters*, Vol. 7, No. 7, July 1974, pp. 515-520.

[10] Beynon, J. H., Saunders, R. A., and Williams, A. E., *The Mass Spectra of Organic Molecules*, Elsevier, New York, 1968, pp. 88-131.

[11] Thornton, J. I. and Fukayama, B., "The Implications of Refining Operations to the Characterization and Analysis of Arson Accelerants. Part II. Chemical Conversions, Treating Processes, and Subsidiary Processes," *Arson Analysis Newsletter*, Vol. 3, No. 3, Aug. 1979, pp. 1-16.

[12] Thornton, J. I. and Fukayama, B., "The Implications of Refining Operations to the Characterization and Analysis of Arson Accelerants. Part I. Physical Separations," *Arson Analysis Newsletter*, Vol. 3, No. 2, May 1979, pp. 1-16.

[13] Smith, R. M., "Arson Analysis by Mass Chromatography," *Analytical Chemistry*, Vol. 54, No. 13, Nov. 1982, pp. 1399A-1409A.

[14] Jackson, M. T. and Walker, J. Q., "Pyrolysis Gas Chromatography of Phenyl Polymers and Phenyl Ether," *Analytical Chemistry*, Vol. 43, No. 1, Jan. 1971, pp. 74-78.

Address requests for reprints or additional information to
R. Martin Smith
Wisconsin Department of Justice Crime Laboratory
P.O. Box 5708
Madison, WI 53705