A Combined Gas Chromatography-Mass Spectrometry-Computer System for the Analysis of Volatile Components of Foods

Charles Merritt, Jr.,* Donald H. Robertson, John F. Cavagnaro,¹ Richard A. Graham, and Thomas L. Nichols

The great complexity in the composition of the volatile components of foods has required the development of elaborate systems of analysis employing the combination of gas chromatography and mass spectrometry for separation and identification. In some laboratories a multiplicity of such analysis systems is employed and a computer becomes a mandatory adjunct in order to process the copious amounts of

One of the primary objectives in studies of flavor chemistry is to establish the chemical composition of the volatile constituents that contribute to the aroma or odor of foods. The role of combined gc-mass spectral methods to perform these analyses is well known. Moreover, the application of computer processing to gc-mass spectral data is likewise becoming well established. Several dedicated gc-mass spectrometry-computer systems are available commercially and a number of configurations for larger computer systems for both on-line acquisition and off-line processing have been described in the literature (Henneberg *et al.*, 1972; Hites and Biemann, 1967, 1968; Knock *et al.*, 1970; Smith *et al.*, 1971; and Venkataraghavan *et al.*, 1970).

The size of a given system and the extent of its use are, of course, largely dictated by the requirements and resources of the user. There is a need, however, to develop means of simplifying the computer systems, reducing their size, enhancing their efficiency, and in particular increasing their utilization by decreasing the cost. This presentation described some approaches which have been devised in our laboratory to achieve some of these objectives.

Although compound identification from mass spectra is possible from basic principles, the identification of unknown compounds from their mass spectra by automatic data processing assumes the existence of a file of data for a large number of known compounds, and the ability to search the contents of that file in a manner which provides component identification. The conventional approach uses tables of mass vs. intensity values that constitute digitized mass spectra. By comparing the unknown to each known spectrum in the library file, and computing a matching index for each trial, it is possible to achieve identification from the best match of the unknown to a known spectrum in the library file.

Because of the large number of spectra to be searched in a gc-mass spectral analysis system, the computer configuration required to execute searches of data for unknown component identification is usually quite large, and the time required for retrieval is slow. Moreover, there is a need in many laboratories to be able to perform computer searches on smaller computers that lack adequate peripheral storage facilities for large data files. data generated. The utilization of a computer for acquiring and processing data from several gcmass spectrometry analysis systems is described with special emphasis on data encoding techniques and procedures for component identification by reference to precoded data files. Examples are given to illustrate the application to typical qualitative and quantitative analyses of volatile food components.

In order to overcome this limitation our laboratory has been concerned with the encoding of spectra in compressed data files. Three different approaches to the construction of such files may be summarized as follows: (1) calculation of entropy function; (2) calculation of divergence function; (3) selected binary encoding.

The first two approaches to the classification of mass spectral data, namely the calculation of the Khinchine entropy function and of divergence values, are derived from set theory, and are based on expressions of the statistical distribution of peaks in a mass spectrum. These as well as the selected binary coding method which is described below all reduce the mass spectrum to a single valued number which is diagnostic for the compound.

The entropy function is expressed as

$$\eta = -\sum_{i}^{n} p_i \log p_i$$

and is calculated by summing the product of the individual ion abundances and their respective logarithms. p represents the ion abundance in terms of the per cent of total ionization of the molecule, or, in another sense, the probability of occurrence of that ion fragment in the spectrum.

Mass spectra are converted by this relationship to a single valued number and in this way a data file can be constructed consisting of these numbers. An example is seen in the portion of such a file tabulated for a group of aliphatic hydrocarbons in Table I. These compounds have been selected to show the typical variation in the entropy value which is expected for the variation in the degree of unsaturation in the molecule. In search of a file of precalculated Khinchine values, a matching index is used to establish the correspondence of the value for an unknown compound with the library value. In early work with Khinchine values, the construction of the reference file was limited to about 200-300 compounds normally encountered in the analysis of volatile components of foods, and in most cases application of the search and retrieval scheme led to single, unequivocal identification of the unknown. In subsequent tests of this procedure with large libraries-e.g., the "Atlas of Mass Spectral Data" (Stenhagen et al., 1969) containing about 7000 compounds-considerable overlap was observed and in many instances there were several compounds which had the same or very close entropy values. Although this may be due in part to the poor quality of the spectral data which exists in most large library files, it has not been possible as yet to purify these data. For libraries of selected compounds, however, the method has been shown to be highly efficacious.

In cases where the entropy values for more than one compound may be too close to provide unambiguous iden-

Pioneering Research Laboratory, United States Army Natick Laboratories, Natick, Massachusetts 01760.

¹ Present address: Department of Chemistry, University of California, Berkeley, Calif.

Table I. Khinchine Entropy Values for Mass Spectra of Selected Hydrocarbons

Compound	Khinchine function
<i>n</i> -Butane	0,927
2-Methylpropene	0.812
trans-2-Butene	1.042
3-Methyl-1,2-butadiene	1.216
1,3,5-Hexatriene	1.340
1,5-Hexadiyne	1.605
3-Heptyne	1.379

Table II. Divergence Values of the Mass Spectra of Selected Hydrocarbons^a

Comparison compd	Divergence, J
<i>n</i> -Hex-1-ene	4.227
2-Methylpent-2-ene	7.780
Cyclohexane	10.024
3-Hexyne	11.830
2-Methylpentene	12.505
1-Hexyne	18.716
2-Hexyne	25.809

^a The reference compound for the series is hexane.

tification, the divergence function is used to resolve the ambiguity (Farbman *et al.*, 1973). The divergence function is expressed as

$$J(1,2) = N_1 \sum_{i}^{n} (p_{1i} - p_i) \ln \frac{p_{1i}}{p_i} + N_2 \sum_{i}^{n} (p_{2i} - p_i) \ln \frac{p_{2i}}{p_i}$$

where

$$p_i = (p_{1i} + p_{2i})/2$$

and N_1 and N_2 are the respective total abundances of ions in each compound.

This function is similar in nature to the entropy function, since the calculation is based on the evaluation of the summation of the products of the ion abundances and their logarithms, but in this case the equation is derived to establish a comparison of the values for two compounds, specifically where p_{1i} and p_{2i} are the ion abundances expressed as the per cent of total ionization for each of the compounds for which the divergence J is calculated. In practice, it has been found convenient to refer the calculation of divergence of a given compound in the aliphatic hydrocarbon series to that of the normal alkane of the same carbon number. Thus, as seen in Table II the divergence values are listed for several C₆ hydrocarbons referred to *n*-hexane. In a like manner, C_4 or C_5 compounds would be referred to *n*-butane or *n*-pentane, C_7 and C_8 to *n*-heptane and *n*-octane, and so forth. Thus, in a library file of divergence values, a group of subsets is established corresponding to the values for the compounds having the same carbon number. This greatly reduces the number of values to be searched and correspondingly the time to execute the search. For example, in the case of two compounds having close entropy values such as hexene and methylpentene, it is seen that divergence values are sufficiently different to provide unambiguous identification.

The calculations required to encode spectra as entropy, and particularly divergence functions, are somewhat lengthy to perform in a small computer without the aid of a hardware arithmetic unit. Moreover, the variability in the values of relative ion abundances with variations in mass spectrometer design and operation produces considerable uncertainty in the reliability of diagnostics based on measurement of spectral intensity factors. For these

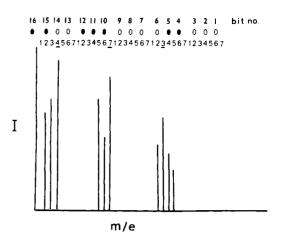


Figure 1. Representation of binary encoding of selected peaks in a mass spectrum.

Table III. Example of Octal Coding

Mass ranges	m/e to be encoded		Binary code	Octal code
23-29	24	2	010	2
30-36	32	3	011	3
37-43	43	7	111	7
44 - 50	0	0	000	0

reasons, there has recently been conceived and tested a codification procedure for use with low resolution mass spectral data banks which allows compression of the library file through selective binary coding of characteristic peaks and use of variable length logical records.

The coding procedure is illustrated in Figure 1. A hypothetical mass spectrum is shown with a representation of a 16 bit computer word at the top. Selective binary coding of characteristic peaks is accomplished by arbitrarily dividing the mass range of interest into multiple groups of seven. The number corresponding to the spectrum peak in each group having the highest intensity is then encoded as a three bit binary number. Thus the fourth peak is encoded in the first grouping, the seventh peak in the second, and so on; zero is used to denote the absence of a peak within the grouping, thereby giving a total of eight possi-ble values, hence the term "octal coding" by which this scheme has been designated in prior descriptions (Robertson et al., 1972). The procedure is quite similar to a method proposed independently by Grotch (1970) in which the spectrum is divided in groups of 14 mass units instead of 7. There are several advantages and disadvantages of grouping of 7 vs. 14, but it is not relevant to discuss those aspects in this presentation. The decision to adopt a grouping of seven in our laboratory was inherently pragmatic since it is based on the word size of our computer.

Representation of an octal number within the computer requires three bits; thus, in a 16-bit machine such as the Hewlett-Packard 2116B used in setting up this system, five octal characters can be stored in each computer word with one bit left over. Thereby a single computer word is capable of storing information which covers a range of 35 atomic mass units. Compounds requiring a greater range of mass units to be encoded require an additional number of computer words. As many are used as are needed to encode the spectrum. The last word is then designated by setting a flag in the 16th bit. A further illustration of the octal coding scheme is seen in Table III.

If consideration is given to the m/e values which occur most often in the spectra of organic compounds, a series of octal ranges beginning with the group of seven masses,

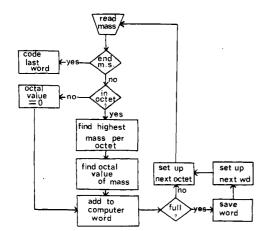


Figure 2. Flow chart for on-line encoding of mass spectra.

Table IV. Subsets of Octally Coded Spectra

No. of words	Subset	
One	Ethane 161000	
Two	Benzene 040371, 160710	
Three	2,3-Dimethyl-3-pentanol 052725, 025252, 102000	

23-29, serves to provide greater diagnostic capability for this method of coding. Subsequent mass ranges would be 30-36, 37-43, etc. The first octad, containing masses 12-14-15-16-17-18-19, was included in the original codification procedures, but when it was learned that no additional information was gleaned from using these m/e values, the entire octad was dropped from consideration.

The efficiency of a coding procedure is reduced by the need to use "0" for coding, *i.e.*, coding which leads to a large number of zeros. If one codes in octads (or some larger sized grouping) there is more likelihood of a peak appearing and thus, according to the basic principles of information theory, provides more efficient transmission of information. In general, the encoding and retrieval of data from a number system such as this are predicated primarily on the principle of simple manipulation of the numbers. By arranging the mass ranges so that certain ions fall characteristically in particular octads, it is also possible to develop qualitative information content as well that may relate to the functional group structure of the molecule. However, presentation of the details of this aspect must be deferred at this time.

The octal code for a mass spectrum may be readily obtained from digitized mass and intensity data acquired on-line and stored for subsequent processing. A flow chart of our program for encoding the mass spectrum into its corresponding octal code words is shown in Figure 2. In our laboratory a normal sequence of data processing would involve the following on-line operations: (1) conversion of the analog mass spectrometer output to digital format, i.e., mass and intensity data; (2) condensation of the data to octal format by means of this routine (Figure 2) which determines the most intense peak in each octal grouping and provides the binary equivalent as the "spectrum" for which the data library is searched; (3) when binary "1" is sensed in the 16th bit, the number of words to encode the "spectrum" is known; thus it is not necessary to search the entire library, but only the subset or sublibrary collection of spectra which require that number of words for coding. With this selective coding technique, it is possible to divide the total file into a series of subfiles based on the number of computer words necessary to selectively code

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Table V. Structure of Library Data File

2	No. of words to encode spectrum
36	No. of compds encoded
$\begin{array}{c} 3040\\ 4000 \end{array}$	Code for MeSH
3	Label for MeSH
$\begin{array}{c} 2570 \\ 0600 \end{array}$	Code for propenal
4	Label for propenal

the spectrum to its highest observed m/e. Some examples are seen in Table IV.

This particular organizational form of the data library file appears to be of special utility in fully automated gas chromatographic-mass spectometric analysis systems, since the highest observed m/e is a quantity readily extracted during the data reduction process. In actual use, such file organization implies prefiltering of the data tables, since only those subfiles having the same number of words as the unknown must be searched.

As previously indicated, the subfiles, as constructed in this work, use the 16th bit of the word to signify the end of the logical record. The word immediately following the end of the logical record thereby contains an integer pointer to a separate file containing the alphanumeric characters of the compound name. The division into subfiles of variable logical record length and creation of a name file were designed to make maximum use of random access mass storage devices. For example, if full binary representation is used to code the spectra of both ethane and tridecane, it is found that sixteen 16-bit words of uniform logical record length are required. However, the use of variable-length logical records for the same pair of compounds requires one and five 16-bit words, respectively, to identify the reference spectra, *i.e.*, ethane and tridecane. An example of the construction of a subset file is illustrated in Table V. The name of the file is designated simply as 2 corresponding to the number of computer words for each compound. The number of compounds in the subset and then the code word(s) for each compound are listed. Instead of listing a name for each compound in the subset which is searched, an index number or label is given for each compound name so that the names can be stored in a separate library and can be called up later without encumbering the computer during a search.

For each unknown compound being searched for in the library, a matching index² is calculated; the five best matches, in decreasing order of goodness of match, are printed. This feature is expected to be most useful in future cases when much expanded library files are being searched and the possibility exists for the same matching index to be calculated for more than one compound.

In addition to the utility of construction of subfiles for more efficient retrieval, the octal coding system is found to provide a damping effect on variations in spectral characteristics due to its relative insensitivity to errors in digitization. For example, errors which may occur in the initial codification of an unknown spectrum, due to a spurious signal or the additive effect of impurities upon peak intensities, have insignificant influence upon correct iden-

² The matching index is calculated in the following way: INDEX = XOR + 2nNZW - 2AND, where XOR is logical exclusive OR and AND is logical AND. XOR = +1 if the *i*th octal window of the unknown disagrees with the *i*th octal window of a library spectrum, and either or both windows are nonzero. XOR = 0 if both windows agree. 2nNZW is twice the number of nonzero windows in the code for the unknown spectrum. AND = +1 if both windows agree and both are nonzero; otherwise AND = 0.

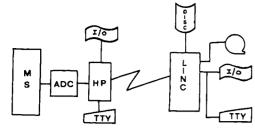


Figure 3. Schematic diagram of computer system.

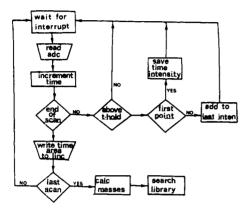


Figure 4. Data flow chart for combined system for acquisition and processing of mass spectra.

tification of the compound in question. Likewise, in the case where the spectrum of an unknown compound is incorrectly coded because of variation in relative intensity values due to mass spectrometer instabilities, it is shown that correct identification may result even in cases where a coding error occurs in each word of the spectrum.

This system of encoding is particularly useful for gcmass spectrometry because only the most intense ions need to appear in the spectrum and trace amounts can be identified even though the less abundant peaks are absent from the spectrum.

The practical application of octal coding to the processing of analytical data for flavor studies is illustrated below. The processing of mass spectral data, however, is constrained by the limitations of the capabilities of the computer system.

A schematic diagram of the equipment available for current studies is shown in Figure 3. The system used for data acquisition is a Hewlett-Packard 2116B computer which is coupled to a gas chromatograph-mass spectrometer analysis system. The mass spectrometer is a magnetic deflection type capable of providing 1-sec spectrum scans which can be digitized by the computer in real time. The system has only 8K of 16-bit core and its I/O structure includes only paper tape read and punch and a teletype. It is thus not possible to output in real time, or to store large volumes of acquired data for subsequent processing. A LINC-8 computer, however, equipped with a disk storage device resides in a nearby laboratory. The LINC-8 is an 8K 12-bit machine having in addition to the disk a paper tape I/O, a teleprinter, and block addressable magnetic tape. By some special output, formatting data from the Hewlett-Packard Computer may be transmitted to the LINC-8 for disk storage of the acquired data. Subsequent processing is then accomplished in the LINC-8.

Figure 4 shows a chart of the data flow in the combined Hewlett-Packard-LINC-8 system. The mass spectrum signal above threshold is digitized and, using centroid computations, is reduced in the Hewlett-Packard to time and intensity values which are transmitted to the LINC in real

Table VI. Composition of Limited Data Library by Function Groups

_				·····
	Alkanes	28	Esters	3 9
	Alkenes	17	Acids	8
	Alkynes	8	Amines	11
	Alkadienes	4	Cyclic	16
	Alkanols	22	Oxy	13
	Alkanals	11	Halogens	4
	Alkanones	18	Thiols	5
		Thiaalka	nes 8	

Table VII. Composition of Word Subfiles in Limited Data Library

No. of words No. of compds	1 9	_	-	-	$5 \\ 22$	•	7 7	8 6	
Total				23	21		-	-	

time and stored on the disk. At the conclusion of a chromatographic run, the spectra are successively retrieved from the disk, mass and intensity are calculated and converted to octal code, and the library is searched. An interim printout can be provided if required by the analyst if, for instance, the spectrum is found not to be in the library and the digitized data are needed for another type of search.

The current system is being used to expedite the interpretation of data obtained from large numbers of samples required to be analyzed by gc-mass spectrometry. In a study of the wholesomeness of irradiated beef the study in 1 year may require identification of the components corresponding to 150,000 spectra. Fortunately, the composition of many of the components can be anticipated and thus a limited library file for searching can be established. Some of the expected compounds in beef as well as other current food items of interest such as strawberries or fish are listed in our current library as shown in Table VI. In all, the library contains about 200 compounds. Using subfiles, however, the number of compounds to be searched in most cases is usually quite limited. Some examples of subfiles from the limited library are shown in Table VII. The top row shows the number of computer words needed to encode the spectrum and the number below corresponds to the number of compounds in the subfile.

An example of a computer search, as executed, to identify a gc peak from an analysis of the volatiles isolated from strawberries is illustrated in Tables VIII-X. A printout of the digitized mass spectrum for scan no. 16, corresponding to one of the peaks in the chromatograms, is shown in Table VIII. The presence of peaks in the spectrum corresponding to masses 18, 28, and 32 can be attributed to background peaks such as water and oxygen and nitrogen from the small amounts of air present. If this spectrum is coded according to the selected mass scheme without eliminating the background, key peaks in the spectrum such as 27 or 31 would not be encoded. It should also be noted that the highest observed mass is 89 which is uneven and probably denotes that the parent mass, which is expected to have an even value, is missing from the spectrum.

An example of a typical computer printout of a library search is depicted in Table IX. In the search routine a method for interaction by the spectroscopist has been established so that one of a number of options may be selected before instituting the search. These options, 1-9, are seen at the beginning of the search routine. In the case depicted here option 4 to delete specific masses is selected, and masses 18, 28, and 32 are eliminated from the spectrum.

Table VIII. Computer Printout of Typical Mass Spectrum of a Gc Eluate (Scan No. 16; Start Time, 906)

Mass	Area
18.0	4,883
27.0	3,125
28.0	22,070
29.0	5,859
31.0	781
32.0	3,125
40.9	2,344
41.9	1,367
43.0	8,594
44.9	977
59.8	1,562
60.8	586
69.9	586
70.9	7,227
72.8	781
87.9	3,125
88.9	586

Table IX. Computer Printout of a Typical Library Search Routine for a Mass Spectrum of a Gc Eluate

Another search? (1 = yes, 0 = no)List the options? 1 Option Operation Read one spectrum 1 2 Subtract one spectrum from another 3 Normalize the spectrum 4 Delete specific masses from the spectrum 5 Delete all masses below a certain per cent of the base peak 6 Octal library search 7 Dump current spectrum 8 Histogram 9 Khinchine library search Option 1 or 2? What scan do you want a library search for? 16 Option 3, 4, 5, 6, 7, 8, or 9? How many? Type the m/e values to be deleted 18 28 32 Option 3, 4, 5, 6, 7, 8, or 9? 6 Search entire library? 0 Search next higher subfile? Strawberry 300KR FD 12/7/72 Scan no. 16; scan time, 906 Matching index Mol wt Compd name

88	2-Methylpropanoic acid	4
88	Ethyl acetate	7
		9
88	Butanoic acid	10
88	2-Methyl-2-butanol	10
116	1-Amyl formate	10

The spectrum of the unknown is then encoded and an octal library search is instituted. Logical zero after the query to search the entire library or higher subfile indicates a NO answer, so only the appropriate subfile is searched corresponding to the number of words in the encoded unknown—in this case a three-word spectrum. The best matches are printed out. The compounds cited do

Table X. Computer Printout of a Typical Library Search Routine for a Mass Spectrum of a Gc Eluate (Continuation)

Hidate (com	(11144 <i>1</i> 1011)	
Another searc	h? $(1 = yes, 0 = no)$	
List the optio	ne?	
0	115.	
Option 1 or 2	2	
1	•	
-	you want a library search for?	
16	you want a notary search ter.	
	, 6, 7, 8, or 9?	
4	, 0, 1, 0, 01 0.	
How many?		
3		
-	values to be deleted	
18		
28		
32		
Option 3, 4, 5	, 6, 7, 8, or 9?	
6	, -, -, -, -	
Search entire	library?	
0		
Search next h	igher subfile?	
1		
Strawberry 30	00KR FD 12/7/72	
-	can time, 906	
, ,	,	Matching
$\operatorname{Mol} \mathbf{wt}$	Compd name	index
116	Ethyl butyrate	1
88	2-Methylpropanoic acid	4
88	Ethyl acetate	7
144	Ethyl N-caproate	7

not fit the data, *i.e.*, mol wt 88 is too low (since the spectrum shows a significantly abundant 89 peak) and 116 is uncertain. Although the higher peaks are missing from the spectrum, it is, nevertheless, rewarding to elect the option of searching the next highest subfile file. This procedure is illustrated in Table X where a logical 1 after the query to search the higher subfile indicates a YES answer. The printout of the search of the four-word subfile shows ethyl butyrate as a good match. In order to corroborate the identification the National Institutes of Health mass spectral data file was subsequently queried *via* a telephone modem and precise agreement with the identification of ethyl butyrate was established.

Butanoic acid

Ethyl N-valerate

2-Ethylhexanol

9

9

9

In summary, octal coding and other single value diagnostics for mass spectra such as entropy or divergence provide for codification of analog mass spectral data in a binary format which facilitates file search for identification purposes by (1) reducing the overall size of data files to be searched and (2) obviating the need for searching the entire file by utilizing variable record length facility to produce subfile classifications.

This method of coding and searching data files for the identification of compounds in gc-mass spectral eluates has greatly reduced the time required to complete the analyses and has eliminated the need to utilize the services of a skilled mass spectroscopist for the interpretation of routine analytical data.

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An Information Acquisition and Utilization System for the Flavor Chemist

William G. Galetto* and William H. Stahl

Most workers in the area of flavor chemistry have collected numerous reprints and/or photocopies of journal articles dealing with various techniques and reports of isolation and identification of flavor components found in natural products. The retrieval of information stored in this fashion soon becomes cumbersome and very time consuming. An information retrieval system has been developed to assist in the utilization of this published information. The total system is com-

Those currently working in the area of flavor chemistry are well aware of the fact that this is an active area of research. There are many academic, governmental, and industrial laboratories involved in flavor work and publishing results of their investigations.

Keeping up-to-date on the voluminous literature, while necessary, can become very time consuming and thus expensive if steps are not taken to facilitate the task. We have developed in our laboratories a system to manipulate the information found in the open literature and present it in a useful printed format.

The total system (Figure 1) is comprised of two major subsystems or data collections: the Journal reference collection and the chemical data collection. These two subsystems are interconnected such that entry anywhere into one leads directly to any information contained within the entire system. All data are handled via low cost programs and in a batch mode, with updating being done two to three times a year. All computer generated reports are in the form of printed directories which can be kept in the laboratories for easy referral or sent to other laboratories if the laboratories are physically separated.

JOURNAL REFERENCE COLLECTION

The journal reference collection subsystem (Figure 2) serves as a means of documenting and retrieving the basic information inherently associated with journal reprints. It is based on a computer program developed by Steed (1971), of Brigham Young University (presently at American River College, Sacramento, Calif.). Data input is via punched cards; output is in the form of printed reports whose contents are represented by the five outer circles

prised of a journal reference subsection (file number, author, key word, reference, and year listings) and a chemical data subsection (where found, name, data, Wiswesser Line Notation, number, and functional group listings). These mesh together to permit entrance at a number of different points. The raw data are manipulated via the computer, resulting in the preparation of a number of directory-type print-outs which are then used directly by the flavor chemist.

shown in Figure 2. The interconnecting arrows indicate the cross-referencing that exists between the various print-outs. The listings can be described as follows. D (file number) is a list, in numerical order, of all journal references in the collection, plus cross-references to authors and journal source data. E-1 (first author) is a listing, alphabetically, by first author; second author, year, file number, and journal source data are included. E-2 (all authors) is an alphabetical listing of all authors; year, file number, and journal source data are included. F (year of publication) is a listing of all references in chronological order; also included are the file number, complete title, and key words. G (key words) is an alphabetical order listing of all key words; file number, year, and full title are referenced. H (reference source) is a listing of journal references in alphabetical order by title of journal; year, first and second authors, and file number are also listed.

The flavorist by referring to one or more of the above six "telephone directory" reports can very quickly learn if any specific paper is in the collection, or, if desired, any and all papers dealing with any specific topic such as raspberry flavor components. The key word file is of particular interest because of its grouping together of papers on the same subject.

MECHANICS OF SYSTEM MAINTENANCE

The article to be added to the system can be in the form of a published paper, thesis, summary, or even an internally generated laboratory report. The number of individual references that can be added is unrestricted. A practical limit, due to running time and print-out size, is estimated at 30,000-50,000 references. This is a number seldom, if ever, approached by the practicing flavor chemist. Very large reference collections could be broken down into smaller subunits and processed separately, if desired.

The actual reprints are assigned a sequential file number as acquired, and in our laboratory are bound in book form in groups of 100. This prevents the loss of reprints

Research and Development Laboratories, McCormick & Company, Inc., Hunt Valley, Maryland 21031.