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Fresh Tomato Aroma Volatiles: A Quantitative Study

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A method for the quantitative analysis of major C_5–C_9 fresh tomato volatiles was developed using Tenax trapping and $CaCl_2$ enzyme deactivation. Information was obtained on the concentrations of (*Z*)-3-hexenal, hexanal, 1-penten-3-one, 2-isobutyl cyanide, 2- and 3-methylbutanols, (*E*)-2-hexenal, (*E*)-2-heptenal, 6-methyl-5-hepten-2-one, (*Z*)-3-hexenol, 2-isobutylthiazole, and 6-methyl-5-hepten-2-ol in fresh ripe tomatoes. The identities of components were confirmed by GC–MS methods. Refrigerator storage (2 °C) of fresh ripe tomatoes was found to lead to a lowering of the concentration of (*Z*)-3-hexenal and other volatiles in the macerated tomato. This provides a scientific basis for the informal subjective observation that such cold storage is deleterious to fresh tomato flavor. It is also of interest in regard to the generally expressed belief that there is a lack of flavor in fresh market tomatoes.

It seems generally accepted that ripe tomatoes, purchased in supermarkets in the United States, lack the desirable aroma and flavor associated with ripe tomatoes picked directly from the plant in the field. There have been a large number of studies carried out on the identification of the volatile flavor components of fresh tomatoes, which have been reviewed (Buttery et al., 1971; Dirinck et al., 1976; Stevens et al., 1977; Wright and Harris, 1985). Despite these (largely qualitative) studies there are some questions unanswered particularly regarding the actual quantitative concentrations of the identified volatile components. Such quantitative data are necessary for the full understanding of the role of the individual components in fresh tomato flavor. One major problem with quantitative analysis has been that some of the enzyme-produced volatile flavor components are themselves degraded by other tomato enzymes before or during the volatile isolation by conventional methods. This was first pointed out by Kazeniac and Hall (1970) who showed that (*Z*)-3-hexenal was largely rearanged to (*E*)-2-hexenal by the tomato medium in about the same order of time needed to isolate the volatiles by the faster conventional methods (ca. 20–60 min).

In the present study we set out to first develop a workable quantitative method for the analysis of the major volatile flavor components of fresh tomatoes and then to apply it to the various forms of fresh tomatoes.

A number of important studies on the nonvolatile flavor (or taste) components of fresh tomatoes have been carried out in recent years (Buesher, 1975; Kader et al., 1978; Stevens et al., 1977).

EXPERIMENTAL SECTION

Materials. Vine-ripened tomato samples were grown on experimental fields in Davis and Albany, CA, during 1985 and 1986. These included the following varieties: Ace, Rutgers, Patio, FM785, Severianin, Oregon II, Ace yellow, and High beta. Fresh market table tomatoes were obtained from local supermarkets. The supermarket varieties were not accurately known but were probably Sunny, Contessa, or related varieties. Unless otherwise stated, tomato samples were stored at room temperature (25 °C) until used.

Authentic reference chemical compounds were obtained from reliable commercial sources or synthesized by established methods. (*Z*)-3-Hexenal was obtained by the CrO_3–pyridine oxidation of (*Z*)-3-hexenol in CH_2Cl_2 following the procedure of Kajiwara et al. (1975). All compounds were purified by gas–liquid chromatography (GLC) separation. This was particularly important for the internal standards 2-octanone and 3-pentanone because small concentrations of impurities in these could interface with the analysis. Ethyl antioxidant 330 (ca. 0.01%) was added to the purified aldehydes, which were stored at freezer temperatures and used within a few hours. Saturated $CaCl_2$ solution was made by adding an excess of $CaCl_2$ to water and then boiling the solution in an open Erlenmeyer flask for 1 h to remove volatile impurities. Diethyl ether (anhydrous) was distilled, and a trace (ca. 0.001%) of Ethyl antioxidant 330 added. It was stored in the dark and used within a few days.

Isolation of Volatile Concentrate from Tomatoes. The tomato sample (100 g at 25 °C) of ca. equal pieces cut from three different tomatoes (of the same lot) was blended (blender blades rotating at 13 670 rev/min) for 30 s. The blended mixture was allowed to stand for 180 s longer, and then saturated $CaCl_2$ solution (100 mL at 25 °C) was added all at once and the mixture blended for 10 s. Five milliliters of a water solution containing 50.0 ppm 2-octanone and 50.0 ppm 3-pentanone was then added and the mixture blended for 10 s. The mixture was then placed in a 1-L flask containing an efficient magnetic stirrer. Purified air (3 L/min drawn from outside the laboratory and passed through activated charcoal) was led into the flask via a Teflon tube and passed over the vigorously stirred mixture and out of the flask through a Tenax trap

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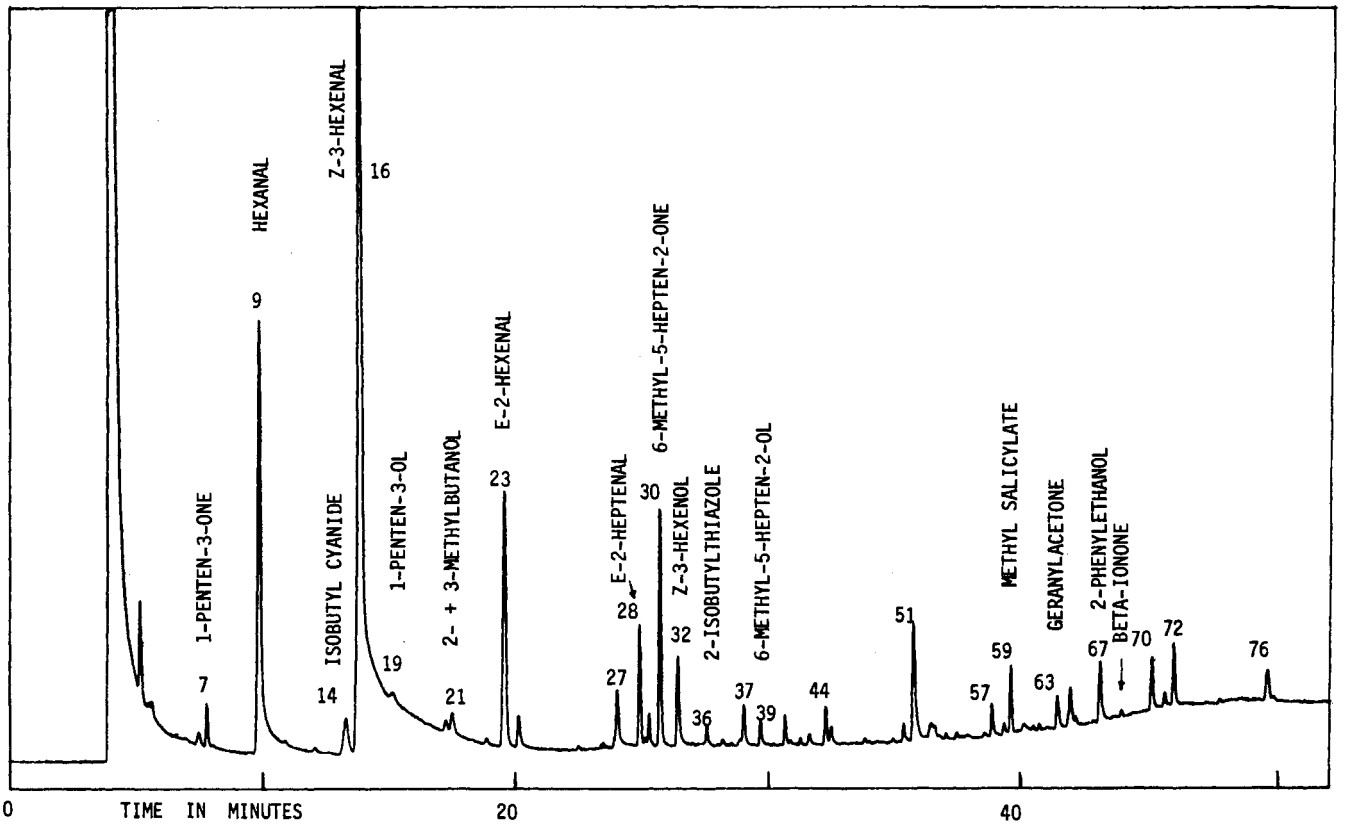

Figure 1. Capillary GLC analysis of the Tenax-isolated volatiles from vine-ripened fresh tomatoes. For GLC conditions see text.

(consisting of a Pyrex tube with standard ball and socket joints at each end and containing a column of Tenax (14-cm length × 2.2-cm i.d.), 10 g). Reduced pressure (ca. 730 mm from an aspirator) was applied to the end of the trap to produce the air flow. All connections were either Pyrex or Teflon. The isolation was continued for 60 min. The trap was then removed and extracted with 100 mL of freshly distilled diethyl ether. The ether extract was then concentrated to ca. 100 μL on a warm water bath and Vigreux distillation columns.

Volatile concentrates were obtained from sliced tomato in essentually the same except that the tomato was cut into ca. 3-mm-thick slices instead of being blended.

Capillary GLC Analysis. The capillary column used for most of the study was a 30 m × 0.25 mm (i.d.) fused silica DB-wax wall coated column. The carrier gas was helium at a flow velocity of 13 cm/s. The GLC oven was held for 15 min at 30 °C after injection, then programmed at 4 °C/min from 30 to 150 °C, and then held at the upper limit. Sample size was 2 μL split 1/20. The injector temperature was 150 °C. The gas chromatograph was a Hewlett-Packard series 5880A with electronic peak area measurement.

Response factors (fid) were determined relative to the internal standards 3-pentanone and 2-octanone by making known solutions in hexane. Relative recovery factors were also determined against the internal standards by making known solutions in water and carrying the mixtures through the isolation and GLC analysis procedures.

Capillary GLC–MS Analysis. This was carried out as described previously (Buttery and Ling, 1985) on a modified Consolidated 21-620 cycloidal type mass spectrometer.

RESULTS AND DISCUSSION

Before quantitative data could be compared between the different tomato samples, it was necessary to develop a workable method for the quantitative analysis of the tomato volatiles. Several methods were tried (including direct solvent extraction and vacuum steel distillation) before the adoption of the final method, described in detail in the Experimental Section. A method was needed that could obtain a quantitative analysis of the volatiles at about the time a fresh sliced tomato might be eaten at its most desirable flavorful stage. The method had to overcome the further enzymatic deterioration of the (enzymatically) initially formed volatiles. This was largely achieved in the present work by incorporating a means to deactivate the enzymes (after the initial formation of desirable volatiles) and by keeping the sampling period relatively short. Because of the difficulties of a completely comprehensive analysis of the whole range of tomato volatiles, it was decided to concentrate the present study on the volatiles in the ca. C_5–C_9 range.

Essentially the quantitative method involved the following steps: (1) blending of the tomatoes and holding the mixture for 3 min to produce the volatiles; (2) addition of saturated $CaCl_2$ solution to deactivate the enzyme systems; (3) addition of internal standards; (4) Tenax trapping of the volatiles by sweeping with a fast air flow; (5) GLC analysis of the Tenax extract. A discussion of the basis of the method and results of testing the method with a model system are outlined later.

GLC–MS analysis was also carried out to verify the identities of all components studied. Figure 1 shows a chromatogram of the volatiles isolated as described. The identities of the compounds are also shown. All compounds had been previously identified by a number of workers [cf. Buttery et al. (1971)]. All major components in the C_5–C_9 range could be identified except for a component labeled "unknown A", which had a retention time between those of (*E*)-2-heptenal and 6-methyl-5-hepten-2-one. The aldehydes (*Z*)-3-hexenal and hexanal form "tailing" peaks on polar stationary GLC phases such as DB-wax, probably due to keto–enol tautomerism. The tautomerism would shift more toward the enol form in

Table I. Comparison of Quantitative Analysis of Volatiles of Blended Samples of Fresh Vine-Ripe (Average Ace, Rutgers, Patio Varieties), Room-Temperature-Ripened (Market) and Green Tomatoes (Ace), and Fresh Sliced Vine-Ripe (Ace) Tomatoes (Concentrations in ppm of Blended Tomato)

compound	vine ripe	room temp ripe	green	vine ripe sliced
2- + 3-methyl-butanal	0.3 (0.1–0.5)[a]	*a*	*a*	*a*
1-penten-3-one	0.5 (0.2–0.9)	0.3	0.03	0.2
hexanal	3.0 (2.0–3.7)	6.1	0.3	0.9
isobutyl cyanide	0.06 (0.01–0.1)	0.1	0.02	0.1
(*Z*)-3-hexenal	12 (9–16)	13	1.6	5.2
2- + 3-methyl-butanol	0.6 (0.2–2)	1.6	<0.005	2.0
(*E*)-2-hexenal	1.1 (0.4–1.7)	1.3	0.13	0.21
(*E*)-2-heptenal	0.05 (0.01–0.1)	0.1	<0.005	0.005
unknown A	0.24 (0.04–0.4)	0.3	<0.005	0.6
6-methyl-5-hepten-2-one	0.16 (0.09–0.3)	0.3	0.02	0.1
(*Z*)-3-hexenol	0.16 (0.08–0.5)	0.16	0.08	2.4
2-isobutylthiazole	0.03 (0.01–.07)	0.01	0.004	0.01
6-methyl-5-hepten-2-ol	0.02 (0.01–0.04)	0.03	0.008	0.008

[a] Concentration could not be determined reliably for 2- and 3-methylbutanals because of solvent peak interference.

(*Z*)-3-hexenal because of the conjugation of the enol (1) and 3 double bonds. A similar situation occurs with phenylacetaldehyde . Nonpolar stationary phases do not give sufficient separation of these two C_6 aldehydes. Unfortunately, the reliable quantitative analysis of 2- and 3-methylbutanals was not always possible because they were frequently obscured by the solvent peak.

Vine-Ripe vs. Room-Ripened and Green Tomatoes. Table I compares the analysis found for blended tomatoes ripened on the plant to those from blended tomatoes purchased from local markets and then ripened for at least 1 week at room temperature. Also shown in Table I are the analyses found for blended green tomatoes and for sliced vine-ripe tomatoes. The results are the averages from at least five samples, and data in parentheses show the range found in samples studied. As might be expected, the concentrations of volatiles found for the green tomatoes were markedly lower than those found for the ripe tomatoes. There did not seem to be much difference, however, between the concentrations found for vine-ripened and room-temperature-ripened supermarket tomatoes, at least for the volatiles in the C_5–C_9 range. We did not find any major differences in the C_5–C_9 volatiles of a number of different types of vine-ripe or room-ripened fresh market type tomatoes (e.g., Rutgers, Patio, Ace, Sunny, Contessa) or process-type tomato (e.g., FM785), although there were some minor differences. We did find significantly lower concentrations of (*Z*)-3-hexenal and hexanal for the vine-ripened fruit in some yellow varieties such as Ace Yellow and High Beta. The Ace Yellow variety also showed a much lower concentration of 6-methyl-5-hepten-2-one, a probably lycopene-derived fragment.

Although a thorough study was not carried out on the compounds larger than ca. C_9, the analysis also showed concentrations of 0.05 ppm for methyl salicylate, 0.03 ppm for geranylacetone, 0.01 ppm for β-ionone, and 0.03 ppm for 2-phenylethanol for the vine-ripe Ace tomatoes.

Tomatoes Stored at Refrigerator Temperatures. Table II lists the concentrations found for tomatoes that had been ripened a week at room temperature and then stored at 2 °C for 7 days. Two types of samples were studied. The samples labeled A were taken directly from the 2 °C refrigerator and blended immediately. The samples labeled B were warmed to room temperature (25 °C) before blending. The temperature was checked by a thermometer inserted into the middle of the tomato. Also shown are data from samples of apparently "ripe" tomatoes obtained directly from a supermarket and analyzed within a few hours with the tomatoes at room temperature (25 °C). The data shown are averages from at least five isolations. Similar results were also obtained with refrigerator storage of vine-ripened Ace tomatoes.

Table II. Average Concentrations (ppm) Found for Volatiles of Ripened Tomatoes Held at 2 °C for 7 Days (Blended at 2 °C (A) and 25 °C (B)) and for Market "Ripe" Tomatoes

compound	ripe A	ripe B	direct market
1-penten-3-one	0.2	0.2	0.2
hexanal	0.23	1.3	1.2
isobutyl cyanide	0.05	0.04	0.2
(*Z*)-3-hexenal	1.3	4.6	3.7
2- + 3-methylbutanols	0.31	0.04	1.2
(*E*)-2-hexenal	0.3	0.17	0.6
(*E*)-2-heptenal	0.01	0.02	0.01
6-methyl-5-hepten-2-one	0.3	0.3	0.09
(*Z*)-3-hexenol	0.02	0.06	0.03
2-isobutylthiazole	0.006	0.01	0.006
6-methyl-5-hepten-2-ol	0.04	0.03	0.02

It can be seen, by comparing Table II with Table I, that the concentrations of hexanal and (*Z*)-3-hexenal are ca. 10 times higher in the room-temperature and vine-ripened tomatoes than they are in those stored at 2 °C and blended without warming. They are ca. 3 times higher than the samples labeled B where the tomatoes were allowed to warm to room temperature before blending. The samples obtained directly from the market showed similar concentrations of the C_6 aldehydes to the cold-storage B samples. Tomatoes kept by supermarkets are usually stored at refrigerator temperatures (after ethylene ripening) to prevent spoilage. It is not surprising then that the concentrations of the C_6 aldehydes for the market and the cold-storage B samples are similar.

It is known (Schwimmer, 1981) that, as for any chemical reaction, the activity of an enzyme system is dependant on the temperature. It is therefore understandable that less of the enzyme-produced C_6 aldehydes are found with the tomatoes blended immediately after removal from cold storage. However, the apparent partial deactivation of the enzyme systems by the storage at 2 °C with the B samples does not seem to have a simple explanation but may be the result of some types of normal tomato metabolism.

(*Z*)-3-Hexenal has been indicated by thorough panel methods to be quite important to fresh tomato aroma (Guadagni et al., 1972; Kazeniac and Hall, 1970). The results in Table II then seem to provide an explanation of why tomatoes purchased at supermarkets lack the flavor of tomatoes ripened on the vine: i.e., because the supermarket tomatoes produce considerably smaller concentrations of (*Z*)-3-hexenal on cutting. This is especially true if the purchaser stores the tomatoes in a refrigerator, which seems to be common practice among the United States public.

Our findings that refrigerated storage leads to a loss of fresh tomato flavor gives scientific support for the informal subjective observation that such cold storage is deleterious to fresh tomato flavor (Lammers, 1981). The findings are also interesting in regard to work carried out by other authors studying cold storage of green tomatoes. Buescher (1975) and Kader et al. (1978) found lower levels of sugars, acids, and total volatiles in the ripe tomatoes if the green

Table III. Odor Thresholds and log Odor Units for Major Volatile Compounds in Sliced Vine-Ripe Ace Tomatoes

compound	odor threshold, ppb	log odor units
(*Z*)-3-hexenal	0.25	4.3
3-methylbutanal[a]	0.2	3.0
β-ionone	0.007	2.5
1-penten-3-one	1	2.3
hexanal	4.5	2.3
(*Z*)-3-hexenol	70	1.5
(*E*)-2-hexenal	17	1.1
3-methylbutanol	250	0.9
2-isobutylthiazole	3.5	0.5
6-methyl-5-hepten-2-one	50	0.3
methyl salicylate	40	0.1
geranylacetone	60	−0.3
(*E*)-2-heptenal	13	−0.4
isobutyl cyanide	1000	−1
2-phenylethanol	1000	−2

[a] Concentration not known with certainty.

tomatoes had been stored at 2–5 °C for some time before ethylene ripening.

Relative Odor Contributions of Components. From the quantitative data found for sliced fresh ripe tomatoes (Table I), it was possible to calculate the number of odor units (U_o) for each of the major compounds. The odor unit was defined by Guadagni et al. (1966) as the ratio of the concentration of the compound divided by its threshold concentration. This value can give some idea of the order of importance of the volatiles to the total odor. Table III lists the major fresh tomato volatiles with their odor thresholds (Buttery et al., 1971) and a calculation of their log odor units in sliced fresh vine-ripe Ace tomatoes. Compounds with the most odor units are listed first. From Table III the major contributors to the odor would be expected to be (*Z*)-3-hexenal, β-ionone, 1-penten-3-one, hexanal, (*Z*)-3-hexenol, (*E*)-2-hexenal, 2- and 3-methylbutanol, 2-isobutylthiazole, and 6-methyl-5-hepten-2-one. Most of these compounds had been suspected to be important previously to the aroma except for 1-penten-3-one. The 2- and 3-isomers of the methylbutanals and methylbutanols have almost the same odor thresholds (and GLC retention times), and only the 3-isomer was listed. The methylbutanal peak was frequently obscured by the solvent peak, and its exact concentration (and hence log odor unit value) is tentative. A water solution of eight of the compounds with the highest log odor units, at ca. the concentrations as listed for sliced tomato in Table I, was judged to be very similar to fresh sliced tomato by a panel of 16 judges.

Development and Testing of Quantitative Method. Partly because or their dynamic nature the volatiles of tomatoes are particularly difficult to isolate and analyze quantitatively. We spent some time developing a workable method, discussed below.

Production of Fresh Tomato Volatiles. The volatiles initially produced by enzyme action when tomato tissue is cut, chewed, or otherwise broken up are the compounds important to the perception of fresh tomato flavor by the consumer. As mentioned earlier however, if the broken tissue is held for too long, further enzyme action takes place that can degrade the compounds first formed. We felt, therefore, for the analysis, that it was necessary to first break the tissue (blending seemed the most uniform and reproduceable method) and hold the broken tissue for a set period (the period 3 min was chosen as it was found that the concentration of (*Z*)-3-hexenal reached a maximum at ca. 3 min). At that point deactivation of the enzyme system would prevent deterioration of the already formed desirable volatiles. Although sliced or diced tomatoes would be closer to the form in which fresh tomatoes are usually eaten, the uniformity obtained by blending was important for the efficient and reproducable isolation of the volatiles. Analysis of volatiles from sliced and diced tomatoes showed lower total concentrations of the same volatile compounds in ca. similar proportions as were found in the blended samples except that the relative concentrations of (*Z*)-3-hexenol and the methylbutanols were generally higher in the sliced and diced tomato.

Deactivation of Enzymes. A number of methods of deactivating the enzyme systems were considered. Schreier and Lorenz (1980) used $CuSO_4$ to deactivate tomato enzymes. Enzyme systems are known to be deactivated by high concentrations of NaCl and other salts (Schwimmer, 1981), and this method was used by Murray and Whitfield (1975) for a number of vegetables. We did not want to use copper or other heavy-metal salts because these are known to react with sulfur compounds and catalyze chemical autoxidation. Saturated NaCl solutions were found to cause some slowing of the change of (*Z*)-3-hexenal to (*E*)-2-hexenal, but use of saturated $CaCl_2$ solutions was found to be considerably more effective. The concentration of (*Z*)-3-hexenal was unchanged after 3 h with $CaCl_2$. The use of bivalent ions such as Ca^{2+} or Mg^{2+} was suggested to us by Schwimmer (1985) as these are effective in precipitating enzyme systems. $CaCl_2$ had also been recently used to deactivate enzyme systems in cucumbers (Geduspan and Peng, 1986).

It is interesting that the common domestic use of salt on sliced tomato (e.g., in a tomato sandwich) would tend to deactivate the enzymes somewhat and thus preserve the concentration of (*Z*)-3-hexenal and hence fresh tomato flavor.

Tenax Trapping of Volatiles. Isolation of volatiles by the now well-known method of Tenax adsorbant trapping provides minimum interference with the blended tomato. Other methods were tried such as vacuum steam distillation and direct solvent extraction but were not as suitable as the Tenax trapping method. The conventional Tenax trap is roughly 0.64 cm in outside diameter and 2.5–7 cm in length (Murray and Whitfield, 1975; Olafsdottir et al., 1985). In previous work with plant volatiles (Buttery and Ling, 1985) much larger traps were used based on calculations of conditions needed to isolate the low concentrations of volatiles found. Model systems of water solutions of typical plant volatiles at room temperature (25 °C) were considered. A flow of gas (air has been used for most of the work) was passed over the stirred solution and then out through the Tenax trap. By simple modifications of some equations developed by Burnett (1963), the total volume (V_a) of sweep gas needed to transfer a percentage (P) of a compound in water solution to the Tenax trap at 25 °C can be calculated

$$V_a = -V_w K^{-1} \ln [(100 - P)/100]$$

where K is the air to water partition coefficient of the compound at 25 °C and V_w is the volume of the water solution. The K value for hexanol is 7×10^{-4} at 25 °C (Buttery et al., 1969), and calculations using the above equation show that ca. 200 L of sweeping gas is idealy needed to sweep 50% of hexanol over to the trap for a solution volume of 200 mL. This is a flow rate of roughly 3 L/min for 1 h. The use of saturated $CaCl_2$ would increase K (the air/water partition coefficient) somewhat by the "salting out" effect, requiring a smaller flow rate of sweep gas for a 50% transfer.

To isolate a reasonable percentage of the volatiles from

Table IV. Percent Recovery from Standard Solutions Compared to 2-Octanone Using the Tenax Isolation Procedure Described in the Experimental Section

compound	% rec[a]	compound	% rec[a]
3-pentanone	46	(*E*)-2-hexenal	75
1-penten-3-one	24	6-methyl-5-hepten-2-one	84
hexanal	67	(*Z*)-3-hexanol	62
(*Z*)-3-hexenal	53	2-isobutylthiazole	89
3-methylbutanol	49	6-methyl-5-hepten-2-ol	93

[a] Corrected for GLC flame ionization detector response factor.

a plant material (within a limited time), it, therefore, seemed that relatively large flow rates of sweeping gas would be needed. Large flow rates required large diameter traps, which also had to be longer to prevent "breakthrough", i.e. elution of the volatiles completely through the trap. Calculations showed, however, that sweep gas velocity through the 2.2-cm-diameter Tenax trap used for the present work with 3 L/min flow rate was of the same order as that used in the common 0.64-cm o.d. (ca. 0.47-cm i.e.) Tenax traps with a flow of 100 mL/min. Air was chosen as the sweeping gas because it was thought that anerobic conditions (e.g., by sweeping with N_2) might produce abnormal volatiles. Good recoveries of aldehyde and terpenoid components showed that no appreciable oxidation occurred on the Tenax (which contains a trace of Ethyl antioxidant 330 left from ether elution). Oxidation is known to occur on other adsorbants such as charcoal. Recovery of the volatiles from the traps with solvent was used because it is more convenient than thermal desorption with such large traps.

Recovery Using Model Systems. To minimize errors in handling and recovery, a measured amount of two internal standards, 3-pentanone and 2-octanone, was added to the tomato medium before the volatiles were isolated. The reasons for using these particular compounds are that they are chemically similar to many of the tomato components, they have retention times not occupied by any significant tomato peaks, and they are relatively stable.

With 2-heptanone as an internal standard added to the final ether concentrate, it was found that an average of 81% of 2-octanone could be recovered from known water solutions under the conditions described in the Experimental Section (including addition of an equal volume of saturated $CaCl_2$ solution). The percent recoveries of other major tomato volatiles relative to that of 2-octanone are listed in Table IV. The recovery seems somewhat related to a compound's affinity for water and hence its volatility (cf. *K*) in water solutions. The absolute recoveries of these compounds are considerably better than those reported by Olafsdottir et al. (1985) who used a more conventional Tenax trapping method. The factors obtained from the percent recovery shown in Table IV were used in calculating the data in Tables I and II.

Preliminary studies with known solutions of compounds larger than C_9 such as geranylacetone and methyl salicylate showed that these also showed a better than 50% recovery under the above conditions.

Accuracy of Results. It is difficult to test the method accuracy with the tomato itself because of the variation within tomatoes of the same lot. Data given in the tables are averages of at least five different isolations. With the known standard solutions of the synthetic compounds in water solution, the average percent deviation from the average of the found concentration with different isolations for the major components was less than 8%.

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Registry No. (*Z*)-3-Hexenal, 6789-80-6; hexanal, 66-25-1; 1-penten-3-one, 1629-58-9; 2-isobutyl cyanide, 625-28-5; 3-methylbutanol, 123-51-3; (*E*)-2-hexenal, 6728-26-3; (*E*)-2-heptenal, 18829-55-5; 6-methyl-5-hepten-2-one, 110-93-0; (*Z*)-3-hexenol, 928-96-1; 2-isobutylthiazole, 18640-74-9; 6-methyl-5-hepten-2-ol, 1569-60-4; 2-methylbutanal, 96-17-3; 3-methylbutanal, 590-86-3; β-ionone, 79-77-6; methyl salicylate, 119-36-8; geranylacetone, 3796-70-1; 2-phenylethanol, 60-12-8; 2-methylbutanol, 137-32-6.

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