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ANALYSIS OF ORGANIC AIR POLLUTANTS
IN THE KANAWHA VALLEY, WV
AND THE SHENANDOAH VALLEY, VA

7

by

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and

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ABSTRACT

Recently developed techniques for sampling and analysis of ambient air by GC/MS/COMP were applied to the Kanawha Valley, WV and Shenandoah Valley, VA to assess the levels of organic pollutants. Volatile and very volatile compounds were concentrated on Tenax GC and carbon sorbent cartridges, respectively, then thermally desorbed directly into the capillary column GC/MS/COMP system for analysis. Semivolatiles were collected on the electrostatic precipitator plates of a Massive Air Sampler, extracted, fractionated, and then analyzed by GC/MS/COMP. The Kanawha Valley contained a broad range of halogenated, ketone, aldehyde, ester, aromatic, aliphatic and polynuclear aromatic compounds. The Shenandoah Valley contained a narrower range of organics, but generally higher observed levels of the compounds quantitated.

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SECTION 1

INTRODUCTION

This study is an outgrowth of a long-term research program to develop and perfect a comprehensive and systematic approach to the measurement of organic compounds in ambient air. Previous research has demonstrated that a wide range of atmospheric contaminants may be readily measured by this technique. Until this technique was developed, the ability to collect and analyze a wide variety of chemical classes from the atmosphere containing toxic and/or carcinogenic compounds was not possible. Thus, the health impact of these compounds had not been thoroughly studied. The techniques used in this study enable the characterization of a wide profile of organic compounds in ambient air. These profiles provided a panoramic view of the pollution at specific sites and times.

Organic compounds are present in the atmosphere at widely varying levels and may be either site-specific or ubiquitous. Sources of these compounds include natural emissions, manufacturing, automobile exhaust, dry cleaning, combustion sources and others. To complicate the milieu, atmospheric reactions degrade some compounds and form others.

The data generated by this technique will allow researchers to identify and quantitate a complex mixture of organic air pollutants in order to begin studying the sources, health effects and environmental effects of these compounds.

SECTION 2

SUMMARY AND CONCLUSIONS

This study was designed to measure a wide range of organic pollutants in two industrialized valleys: the Kanawha Valley, WV and the Shenandoah Valley, VA. The Kanawha is heavily industrialized with a wide variety of chemical industry stretching for roughly 40 km. The valley is narrow with high hills providing a well-defined emission reservoir. The metropolitan population is roughly 150,000. Sampling locations were selected at various sites throughout the valley to assess the general levels of organic compounds. In contrast, the Shenandoah is heavily reliant on tourists and its only major chemical industries are a viscose rayon plant and an allied sulfuric acid plant. The valley is broad and ill-defined near Front Royal (population about 10,000) and would not be expected to trap pollution to any great extent. Sampling sites were selected both upwind and downwind of the industrialized area, and in the center of town in order to assess pollution levels in the area.

Very volatile organic compounds in ambient air (e.g., vinyl chloride) were concentrated on carbon cartridges. Volatile organics (e.g., acetone through naphthalene) were collected on Tenax GC sorbent cartridges. Typical sampling volumes for both carbon and Tenax GC samples were 200-600 l of air. Semivolatiles (e.g., polynuclear aromatics) were collected as particulate using a Massive Air Sampler which collected the $<1.7 \mu$ respirable particulate fraction of interest on electrostatic precipitation plates. Typical particulate sampling volumes were 20,000-90,000 m³.

The volatile and very volatile compounds collected on the sorbent cartridges were analyzed by thermal desorption in line with a gas chromatograph, mass spectrometer/computer (GC/MS/COMP). High resolution was achieved using an SE-30 SCOT capillary column. The semivolatile compounds were extracted from the particulate, fractionated and then analyzed by capillary

column GC/MS/COMP. Data were interpreted by comparison with known mass spectra from spectral libraries. Selected compounds in the volatile fraction were quantitated using the intensities of selected mass ions.

The volatile compounds identified in the Kanawha Valley (with the number of times observed out of ten samples interpreted) include: vinylidene chloride and/or the dichloroethylene isomer (8), methylene chloride (10), chloroform (10), 1,2-dichloroethane (2), 1,1,1-trichloroethane (8), 1-chlorobutane (1), carbon tetrachloride (8), dichloropropene (1), trichloroethylene (6), 1,2-dibromoethane (2), tetrachloroethylene (9), chlorobenzene (1), dichlorobenzene (8), acetaldehyde (9), benzaldehyde (9), aliphatic aldehydes (11), acetone (10), acetophenone (7), benzophenone (4), 21 other ketones, ethyl acetate (6), seven other esters, isopropanol (2), phenol (7), six other alcohols, diethyl ether (5), diphenyl ether (4) and eight other ethers, benzene (9), alkyl benzene, indan (7), indene (1), naphthalene (8), alkyl naphthalenes, biphenyl (7), CS₂ (6), other sulfur-containing compounds, cyanobenzene (1), C₃-alkyl pyridine (1), and many alkanes. Quantitative results included high values of 334 ng/m³ for methylene chloride, 1536 ng/m³ for tetrachloroethylene, and 71,778 ng/m³ for benzene. Compounds identified in the particulate fraction included long-chain alkanes, polycyclic aromatic hydrocarbons (PAH) from naphthalene through anthanthrene (or an isomer), alkyl-PAH derivatives, and nitrogen-containing heterocycles.

In the Shenandoah Valley, VA, the volatile compounds identified (with the number of times observed out of nine samples interpreted) include: vinylidene chloride and/or the dichloroethylene isomer (9), methylene chloride (9), chloroform (9), 1,2-dichloroethane (1), 1,1,1-trichloroethane (3), carbon tetrachloride (6), trichloroethylene (3), tetrachloroethylene (6), dichlorobenzene (5), acetaldehyde (9), benzaldehyde (6), nine aliphatic aldehydes, acetone (9), acetophenone (6), benzophenone (2), three other ketones, ethyl acetate (4), phenol (5), five alkyl phenols, diethyl ether (8), benzene (8), alkyl benzenes, indan (5), naphthalene (6), alkyl naphthalenes, biphenyl (3), and alkanes. Quantitative results include high values of 238,000 ng/m³ for methylene chloride, 14,500 ng/m³ for chloroform, 2,933 ng/m³, 1,1,1-trichloroethane, 2,994 ng/m³ for

tetrachloroethylene, 24,000 ng/m³ for benzene, and 3,721 ng/m³ for acetophenone. Semivolatile compounds identified included polycyclic aromatic hydrocarbons (PAH) from naphthalene through C₂₂H₁₂, alkyl-PAH derivatives, oxygenated PNAs, (ketone and anhydrides), sulfur heterocyclic PNAs, and aliphatic hydrocarbons.

Many more compounds were identified with greater frequency in the Kanawha Valley than in the Shenandoah Valley. This is especially noticeable in the pollutants potentially arising from industrial activity (halogenated and oxygenated compounds). Many compounds, including the aromatics, result from combustion (e.g., automobile exhaust) or other sources which could be considered ubiquitous. This qualitative comparison is in keeping with the greater industrial diversity and higher population density of the Kanawha Valley.

In contrast to the qualitative data, the quantitative data showed much higher levels of most organic pollutants in the Shenandoah Valley than in the Kanawha Valley. This is especially noteworthy, since the Shenandoah Valley is broader and well-defined and is therefore not expected to be as good an emission reservoir as the Kanawha Valley. The high levels in the Shenandoah Valley were found on both Trips 1 and 2, implying that the levels found are not fortuitous.

SECTION 3

RECOMMENDATIONS

The results of this study indicate the widespread occurrence of organic compounds in ambient air in these two valleys, sometimes at higher levels. Further research may be directed along eight major fronts:

(1) More vigorous sampling protocols could hopefully identify point source polluters for possible regulatory action.

(2) Long-term monitoring of these valleys may provide both mean concentration data and show any trends in levels of compounds. This data could be useful in identifying industrial pollutants and in establishing a data base for future epidemiological studies.

(3) Future studies could integrate this type of air monitoring with sampling and analysis of other media including water, sediment, soil, vegetation, human tissue, mothers milk, etc.

(4) Future studies should more comprehensively study the correlation of meteorology with pollutant levels (i.e., Do concentrations of specific pollutants rise during an inversion?).

(5) Epidemiological studies could begin to attempt to correlate disease incidence (e.g., cancer) with levels of toxic and/or carcinogenic compounds in air and other media to which humans are exposed.

(6) Expansion and perfection of the techniques reported herein could present a more complete picture of the pollution in these valleys.

(7) More research along the lines of this study and the recommendations given above is needed to fully characterize the air pollution associated with industrialized valleys. Future studies should include both industrialized, residential/commercial, and uninhabited valleys. In addition, more samples taken over longer time periods are needed to accurately assess pollutant levels.

(8) Since it appeared that the highest concentrations of some pollutants may have occurred at night, it may be important in future studies to integrate the samples for at least 24 hr and/or take consecutive samples which cover entire 24 hr periods.

SECTION 4

OBJECTIVES

This study was designed to provide information on the general organic air pollutant levels in two industrialized valleys. In specific:

- (1) Samples were to be collected at three monthly intervals to assess changes of pollutant levels with time.
- (2) Samples were to be collected at locations selected to show general pollutant levels in the valley, especially the levels effecting the human population.
- (3) Samples were to be analyzed by gas chromatography/mass spectrometry/computer to provide accurate and positive identification of the compounds present.
- (4) Qualitative and quantitative data were to be presented such that EPA, Region III personnel could determine the extent to which organic chemicals may affect the human population in the areas sampled.

SECTION 5

SAMPLING

SAMPLING EQUIPMENT

Due to the wide range of compounds sought, it was necessary to use more than one collection method. Highly volatile compounds were collected on carbon cartridges. Compounds of medium volatility were collected on a polymeric sorbent cartridge (Tenax GC). Particulates were collected on impactor and electrostatic precipitation plates using an ultra-high volume Massive Air Sampler (MAS).

Collection of High- and Medium-Volatility Organics on Carbon and Tenax GC

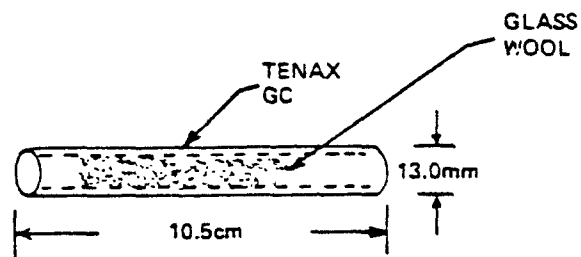
High and medium volatility materials were concentrated from ambient air on a sampling train consisting of (1) a glass fiber filter (GFF), (2) a cartridge of Tenax GC, and (3) a cartridge of carbon, sequentially.

Glass Fiber Filter (GFF)--

As illustrated in Figure 1, the glass fiber filter (GFF) was placed at the front end of the sampling train, held in place by a 25 mm Delrin filter holder. Gelman Type A-E 25 mm diameter filters were used. These filters are rated at 99.7% efficiency for particles greater than 0.3 μm by the dioctyl phthalate permeation test, and at 98% efficiency for particles of 0.05 μm diameter or larger. The filter was used primarily to exclude particulate containing non-desorbable compounds which would contaminate the Tenax GC.

A series of experiments were conducted to determine whether the GFF excluded chromatographable compounds from the Tenax GC cartridge. Parallel cartridges, with and without the GFF, were sampled near a highway intersection with a large number of diesel trucks starting and stopping (U. S. 70 and Old U. S. 70, Bethesda, NC). Gas chromatographic analysis with flame ionization detection (GC/FID) of these two cartridges yielded similar gas

GLASS CARTRIDGE SAMPLER



VAPOR COLLECTION SYSTEM

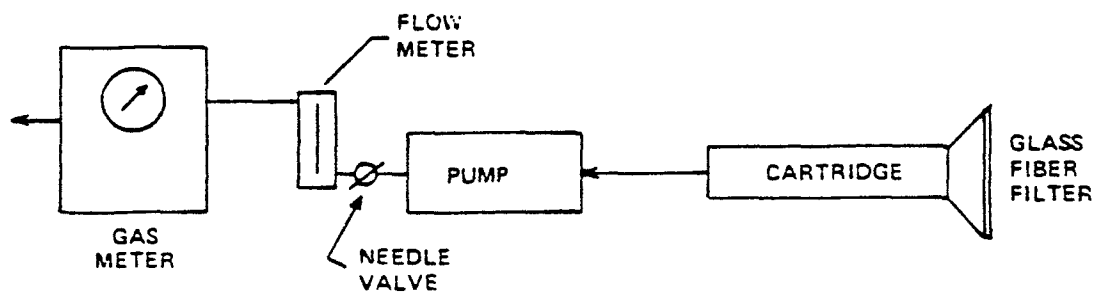


Figure 1. Collection system for concentrating high and medium volatility organic compounds from ambient air.

chromatograms, indicating no desorbable compounds were being excluded from the Tenax GC cartridge by the GFF. Based on these results, the GFF was retained in the sampling train, since its use allowed recycling of the Tenax GC resin.

Tenax GC Sampling Cartridges--

The sampling tubes were prepared by packing a 10 cm x 1.5 cm i.d. glass tube containing 6.0 cm of 35/60 mesh Tenax GC (1.6 g) with glass wool in the ends to provide support.⁽¹⁻³⁾ Virgin Tenax GC was extracted in a Soxhlet extractor for a minimum of 18 hours with acetone prior to preparation of cartridge samplers.^(1,2) In those cases where sampling cartridges of Tenax GC were being recycled, the sorbent was extracted in a Soxhlet apparatus with acetone, as described for the virgin material, and also extracted with a non-polar solvent, hexane, in order to remove the relatively non-polar and non-volatile materials which might have accumulated on the sorbent bed during previous sampling periods.

After purification, the Tenax GC was meshed to provide a 35/60 particle size range. Cartridges were then prepared and conditioned at 270°C with helium flow at 30 ml/min for 20 minutes. The conditioned cartridges were transferred to Kimax[®] (2.5 cm x 150 cm) culture tubes, immediately sealed using Teflon-lined caps, and cooled. This procedure was performed in order to avoid recontamination of the sorbent bed.^(1,2) One or more cartridges selected at random from each batch were checked for background using GC/FID. If the background was unacceptable, the cartridges were redesorbed and checked again.

For large sample volumes it is important to realize that elution of certain organic compounds through the sampling tube will occur if their breakthrough volume is exceeded. The breakthrough volume is defined as that point at which 50% of a discrete sample introduced into the cartridge is lost. The breakthrough volumes of some representative compounds are shown in Appendix A.^(1,2,4,5,6) These breakthrough volumes have been determined by a previously described technique.^(1,4) Although the identity of a compound during ambient air sampling is not known (therefore, also its breakthrough volume) the compound can still be quantitated after identification by GC/MS/COMP once the breakthrough volume has been established.

Thus, the last portion of the sampling period represents the volume of air sampled prior to breakthrough. For cases when the identity of the compound is not known until after GC/MS/COMP analysis, the breakthrough volume is determined after the fact and the quantitation accomplished as above.

Previous experiments have shown that organic vapors collected on Tenax GC sorbent are stable and can be quantitatively recovered from the cartridge samplers up to four weeks after sampling when they are tightly closed in cartridge holders, protected from light, and stored at 0°C.⁽¹⁾

Carbon Cartridges--

High purity charcoal (SKC, Inc., Pittsburgh, PA) was packed into a bed, 3 x 0.3 cm, in a glass tube. Carbon from this source has been shown to be pure for these applications and was used without solvent purification. Carbon cartridges were thermally stripped of organic vapors by heating to 400°C under He flow for 30 min.

These cartridges efficiently trap the organic compounds which pass through the Tenax GC cartridge (vinyl chloride, vinyl bromide, methyl chloride, and methyl bromide). They have been successfully used to analyze vinyl chloride and the other highly volatile halocarbons (b.p. <30°) which are not retained on Tenax GC to any significant extent.⁽⁷⁾ The breakthrough volume for vinyl chloride, and thus the amount collectable, on the carbon cartridges is about 20 times that of Tenax GC.

Sampling Apparatus--

Continuous sampling of ambient air was accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Figure 1). The flow was monitored through a calibrated rotameter, and the total flow registered by a dry gas meter. Concomitant with these parameters, the temperature was also noted, since it was important for establishing the breakthrough volume and therefore the total sampling volume which can be used for quantitation. This portable sampling unit operated on a 12-volt storage battery and was operated from 4-12 hrs, depending on the sampling conditions and flow rates used. Duplicate cartridges were deployed on each sampling unit. A total of four portable sampling units were available for sampling.

At the same location as the MAS (vide infra), a duPont Model P-200 personnel sampler was used to continuously sample air onto carbon and Tenax GC cartridges over the entire period that the MAS was operated. The duPont personnel sampler, operated at about 200 cc/min, was powered by a 6V lantern battery and the entire sampler housed in a chrome-plated aluminum box.

Collection of Low-Volatility Organics Using a Massive Air Sampler (MAS)

A Massive Air Sampler (MAS) manufactured by Battelle Memorial Institute, Columbus, OH^(8,9) was used for collecting particulate fractions in the 3.5 - 20, 1.7 - 3.5 and <1.7 micron ranges. Preliminary studies (personal communication R. Burton, Environmental Assessment Branch, HERL, USEPA, RTP, NC) indicated that the larger particle range yielded greater than 1 g in a 100 hr collection period at an 18 m³/min sampling rate. The middle sized particle range was found to be approximately 0.8 g while the smallest particles were well over 3 g for this collection period and rate.

The sampler, about 140 cm tall and 60 cm square, is a large cascade impactor with electrostatic precipitation for collection of the fine particulate which is not impacted. Air is sampled at a rate of 630 cfm (18 m³/min) by a blower using a 750j/sec motor (115 V, 12 amps). The air enters the sampler over a lip enclosed by the cover which serves as a scalping stage with a cutoff of about 20 μ . The air then enters the impactor assembly stages consisting of four Teflon-coated plates (28 x 43 cm). The first and third plates have slots which serve as impactor jets. The second and fourth plates are the collection target plates located about 1 cm below the jet plates. Below the impactor sections is the electrostatic precipitator, consisting of ionizing wires (-10 kV) and 55 Teflon-coated collection plates (28 x 43 cm). The plate potential is adjusted to the maximum achievable without excessive arcing (generally 5-7 kV, depending on the humidity). From the electrostatic precipitation section, the air is drawn to the blower and then to exhaust. The control panel consists of a magnahelic vacuum gauge to register the flow, a run time meter (in hours), a volt meter to indicate the voltage applied across the precipitator plates, and a red flashing light to indicate malfunctions.

For the purpose of this study, the MAS was chained into a pickup truck for transportation and left in situ during sampling.

Upon return from the field, the impactor and electrostatic precipitator plates were scraped into glass vials, kept in the dark, and stored under nitrogen at -5° to retard chemical reactions. The plates were scraped in a specially designed glove box to prevent contamination of the sample and for protection of personnel.

METEOROLOGY

Continuous measurements of temperature, wind direction and wind run were recorded on a MRI (Meteorological Research, Inc. Altadena, California) Mechanical Weather Station (MRI) at a central location through the sampling period. The strip chart record allowed subsequent reference to calm periods, wind direction shifts, etc., which could affect sampling results. Intermittent measurements were made at each sampling location. Humidity, temperature, wind speed, and wind direction were measured and noted along with general conditions (rain, snow, cloud cover, odors, etc.). Measurements at each location provided a cross-check with the MRI record.

Pertinent meteorological data for the sampling period were obtained from the nearest National Weather Service office. This data was used to augment that obtained at the sampling location.

SAMPLING PROTOCOLS

Samplers were set out at locations designated in a numerical sequence (e.g. L1) for a sampling period (e.g. P1). Thus, each sample is designated by a unique Trip/Period/Location (e.g. Trip 1, P2/L6) code. This code is presented in the sampling protocol tables and then used to identify samples in the analytical results.

SAMPLING LOCATIONS

Kanawha Valley

Many manufacturers of organic chemicals which, along with the by-products, are potentially toxic, carcinogenic and/or teratogenic are located in the Kanawha Valley, W.V. (Figure 2). DuPont, near Belle, has a large chemical complex for the synthesis of substances such as methyl-methacrylate, methylamines, ammonia, hydrogen cyanide, herbicides, and insecticides. In South Charleston are production and consumption plants (Union Carbide,

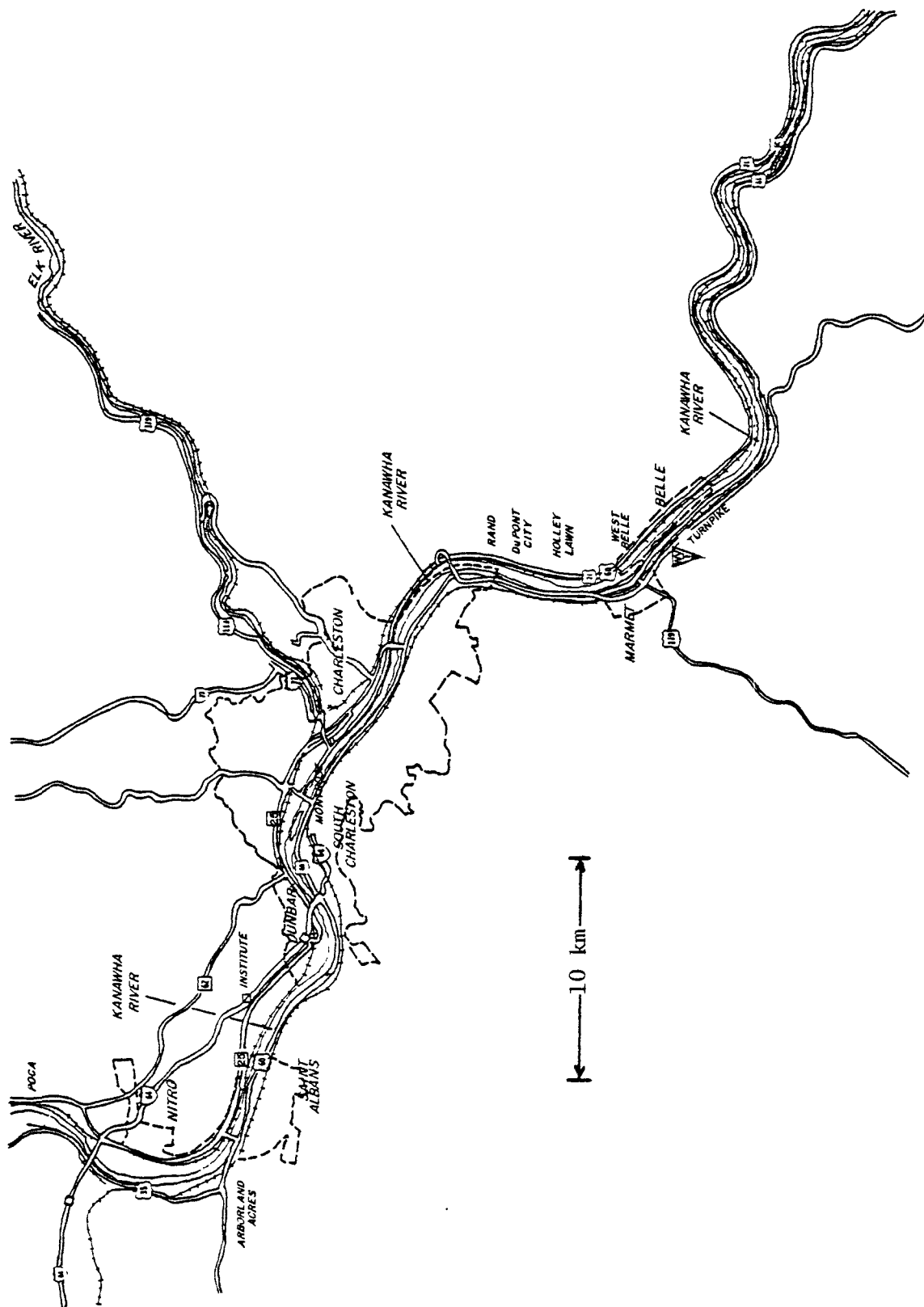


Figure 2. The Kanawha River Valley, West Virginia.

and FMC). Plastics, PVC, antifreeze, chlorine, halogenated organics, carbon disulfide, peroxides, etc. are the predominant chemicals produced here. The major facility in the town of Institute is Union Carbide which also processes a broad spectrum of compounds, e. g., viscose rayon, and phthalate esters. There is also a large scale olefin processing complex and a rubber accelerator plant. A major terminal loading facility in South Charleston handles large quantities of a variety of organic compounds. Monsanto, FMC, Allied, and Fike have plants near Nitro for the production of antioxidants, rubber accelerators, industrial chemicals, and other materials. Several other chemical manufacturers, consumers, and transporters are located in the Kanawha Valley, some or all of which may contribute to the presence of organic materials in the ambient air.

Previous sampling and analysis efforts have found a wide variety of organic compounds in ambient air.^(1,10,11) These results were used in part to select locations for sampling during this study.

The rationale for selection of the locations in the Kanawha Valley was to place samplers at several points along the valley floor throughout the industrialized, metropolitan Charleston, WV area. The location was selected within a general area by sampling personnel on the basis of estimates on where high concentrations of air pollutants might be detected, the potential for human exposure, security of personnel and equipment, and also approval of property owners where applicable.

The MAS, duPont sampler, and MRI weather station were located at the North Charleston Community Center (21st St. W. and 7th Ave., W.) based on recommendations from personnel in the Environmental Assessment Branch, HERL, EPA, RTP, NC who had sampled there previously with the MAS. This location provided not only power, but fenced-in areas for security. Centrally located in the valley, this location was judged to provide "average" meteorology and air samples.

The other four samplers were located up and down the valley at locations in Belle, South Charleston, St. Albans or Institute, and Nitro.

The sampling locations, times, volumes, and meteorology are summarized in Tables 1-4. The location numbers are shown on detailed maps (Figures 3-6).

Table 1. SAMPLING LOCATIONS IN THE KANAWHA VALLEY, WV.

Location	Site	Address	Remarks
L1	Charleston	4th Ave. W. and 21st St. W.	North Charleston Recreation Center. [MAS located at Maintenance Steel near west entrance; MRI and duPont samples located around swimming pool.
L2	S. Charleston	314 4th Ave.	S. Charleston Fire Department Sample located on upper level roof.
L3	St. Albans	6500 MacCorkle Ave. S.W.	Riverside Nursing Home. Sampler located on river bank in open area.
L4	Nitro	N.W. of intersection of W.V. 25 and I-64.	Nitro Sewage Treatment Plant. Sampler located along fence, upwind of all sewage treatment facilities.
L5	W. Belle		Marmet Dam and Locks. Sampler located on hill above parking lot.
L6	Nitro	2009 20th St.	Nitro Fire Department. Sampler located on roof.
L7	Nitro	4107 1st Ave.	Front yard of private residence, directly across street from chemical manufacturing facilities.
L8	Institute	Barron Dr. between 4th St. and Curtis Sq.	Back yard of private residence.
L9	Nitro	N.W. of intersection of W.V. 25 and I-64.	South side of United Distribution Service parking lot.

Table 2. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN
KANAWHA VALLEY, WV ---- TRIP 1

Site	Period/Location	Sampling Time	Sampling Volume (l)	Remarks ^a
Charleston	P1/L1	1030-1435 (9/27 - 9/28)	29,500,000 ^a	^b T = 7°C to 20°C. Winds: S.S.W. to W./calm to 2.8 m/s.
Charleston	P1/L1	1020-1435 (9/27 - 9/28)	258 ^c	At 0955 (9-27), RH ^d = 85%, T = 19°C, low cloud cover.
S. Charleston	P1/L2	1115-1617	597	T = 22°C, RH = 72%, low cloud cover.
St. Albans	P1/L3	1202-1715	557	T = 17°C to 20°C. Winds: S.S.W. to W.S.W./1.4 to 2.8 m/s. Rain for 1 hour.
Nitro	P1/L4	1400-1610	497	T = 18°C to 20°C. Winds: S.W./1.7 to 2.8 m/s.
W. Belle	P1/L5	1349-1945	564	T = 18°C to 20°C. Winds: S.W./1.7 to 2.8 m/s.
S. Charleston	P2/L2	0825-1308	558	T = 8°C to 13°C. Winds: W. to S.W./0.5 to 1.7 m/s.
St. Albans	P2/L3	0715-1355	710	T = 8°C to 15°C. Winds: W. to S.W./calm to 1.7 m/s.
W. Belle	P2/L5	0740-1555	541	T = 7°C to 20°C. Winds: W. to S.W./0.5 to 1.7 m/s.
Nitro	P2/L6	0930-1320	410	T = 9°C to 13°C. Winds: W. to S.W./1.1 to 1.7 m/s; overcast.

^aSample collected with MAS

^bTemperature

^cLong-term samples taken with small duPont personal sampling pump.

^dRelative humidity

^aGeneral weather conditions for 9/27 and 9/28: Cool, skies overcast with periods of intermittent light rain and slow but steady showers.
Winds: calm to light breezes.

Date: 9/27-28/77

Table 3. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR IN
KANAWHA VALLEY, WV ---- TRIP 2

Site	Period/Location	Sampling Time	Sampling Volume (L)	Remarks*
Charleston	P1/L1	0910-0820 (10/24-10/26)	49,700,000 ^a	T ^b = 7°C to 23°C, RH ^c = 31% to 91%. Wind: E.S.E./ calm to 7 m/s.
Charleston	P1/L1	0925-0850 (10/24-10/26)	512 ^d	At 0910 (10-24), T = 10.5°C, RH = 87%, partly cloudy. Eight hours of light rain during sampling time T = 13°C to 22°C ^e , RH = 35% to 93%. Winds: E.S.E. to E.W./calm to 6 m/s ^f .
S. Charleston	P1/L2	1200-1737	268	T = 23°C to 18°C. Winds: S. to E.S.E./1.1 to 5 m/s. At 1151, T = 23°C, RH = 32%, slightly hazy, no odors.
St. Albans	P1/L3	1130-1635	370	T = 17°C to 23°C. Winds: S.S.W. to E.S.E./1.1 to 5 m/s. At 1125, T = 17°C, RH = 54%, low haze, no odors.
Nitro	P1/L4	1035-1600	322	T = 17°C to 23°C. Winds: S.S.W. to E.S.E./1.1 to 5 m/s. At 1030, T = 17°C, RH = 68%; hazy, strong odor.
W. Belle	P1/L5	1315-1808	414	T = 23°C to 17°C. Winds: S.S.W. to E.S.E./1.1 to 5 m/s. At 1313, T = 23°C, RH = 50%; hazy, slight odor.
S. Charleston	P2/L2	0632-1205	297	T = 14°C to 18°C. Winds: E. to S.E./calm to 4 m/s. RH = 58% to 69%.
St. Albans	P2/L3	0534-1147	432	T = 14°C to 18°C. Winds: E. to S.E./calm to 4 m/s. At 0533, T = 14°C, RH = 88%; overcast, strong odor. RH = 55% to 72% ^f .
Nitro	P2/L4	0505-1118	410	T = 14°C to 17°C. RH = 55% to 72% ^f . Winds: E. to S.E./calm to 4 m/s. Overcast, strong odor. At 0505, T = 18°C ^e , RH = 79%.
W. Belle	P2/L5	0600-1235	569	T = 13°C to 18°C. RH = 55% to 72% ^f . Winds: E. to S.E./calm to 4 m/s. At 0555, T = 13°C. Overcast, no odor. RH = 69% to 54%.

^a Sample collected with MAS.

^b Temperature.

^c Relative humidity.

^d Long-term sample collected with duPont personal sampling pump.

^e Temperature beside sewage treatment plant settling ponds -- somewhat higher than ambient.

^f Data from National Weather Service Forecast Office, Kanawha Airport, Charleston, WV.

* General weather conditions for 10/24 through 10/26. Cool, clear, overcast.

Table 4. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR
IN KANAWHA VALLEY, WV --- TRIP 3

Site	Period/Location	Sampling Time	Sampling Volume (L)	Remarks ^a
Charleston	P1/L1	1910-0917 (11/16-11/20)	90,800,000 ^a	Odors: occasionally strong chemical. At 1005 (11-17) RH ^e = 63%. At 1125 (11-18) RH = 38%. T ^c = 2 to 15°C ^f , RH = f 28% to 100% ^f . Winds: S.W. to N. to E. f/calm to 11 m/s. f T = 4°C to 15°C ^f , RH = 31%-80% ^f . Winds: S. to W./2-11 m/s. f
Charleston	P1/L1	1910-1125 (11/16-11/18)	344 ^b	
S. Charleston	P2/L2	1235-1737	1087	T = 11°C to 9°C. Wind: W.S.W./6 to 10 m/s. RH = 31% to 44% ^f .
W. Belle	P2/L5	1348-1811	1205	T = 11°C to 9°C. Wind: W.S.W./4 to 10 m/s. RH = 31% to 44% ^f .
Nitro	P2/L7	1335-1725	480 ^d	T = 11°C to 10°C. Wind: W.S.W./4 to 10 m/s. At 1335 and 1720, odor strong. RH = 31% to 44% ^f .
Institute	P2/L8	1235-1700	861	T = 11°C to 10°C. Wind: S.W.S./6 to 10 m/s. At 1235 and 1700, odor acrid, of rotting walnuts. RH = 31% to 44% ^f .
Charleston	P3/L1	1135-0930 (11/18-11/20)	331 ^b	At 1125 (11-18), T = 10°C, RH ^e = 38%, sky clear. T = 1°C to 15°C ^f RH = 28% to 100% ^f . Wind: S.W. to N. to E. f/calm to 6 m/s ^f .
S. Charleston	P3/L2	0809-1310	1096	T = 4 to 9°C ^f , RH = 49% to 33% ^f . Wind: W.S.W. f/4 to 8 m/s ^f .
W. Belle	P3/L5	0729-1241	1084	T = 4 to 9°C ^f , RH = 49% to 33% ^f . Wind: W.S.W. f/4 to 8 m/s ^f .
Institute	P3/L8	0728-1210	743	Odor of rotting walnuts, naphthalene or mothballs. T = 4 to 9°C ^f , RH = 49% to 33% ^f . Wind: W.S.W. f/4 to 8 m/s ^f .
Nitro	P3/L9	0802-1250	953	Strong odor. f T = 4 to 9°C ^f , RH = 49% to 33% ^f . Wind: W.S.W. f/4 to 8 m/s ^f .

^a Sample collected with MAS

^b Long-term sample collected with duPont personal sampling pump.

^c Temperature

^d Pump malfunctioned during sampling period.

^e Relative humidity.

^f Data from National Weather Service Forecast Office, Kanawha Airport, Charleston, WV.

* General weather conditions for 11/16 through 11/20: Temperatures cool. Skies clear to partly cloudy with very small amount of rain. Winds very brisk with occasional gusts, diminishing to calm on 11/20.

Dates: 11/16-20/77

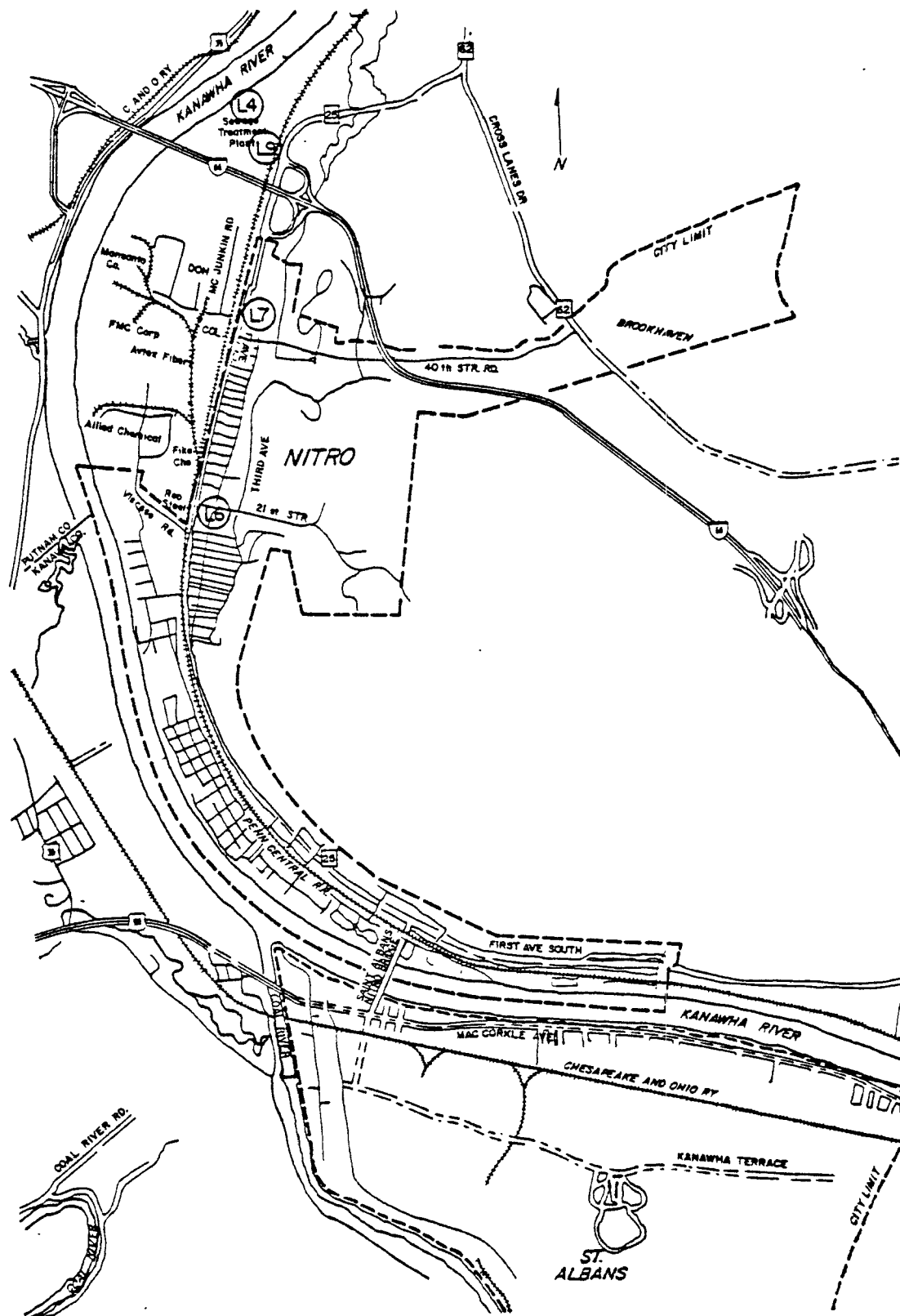


Figure 3. Map of area around Nitro, WV showing L4, L6, L7, and L9 (See Table 1).

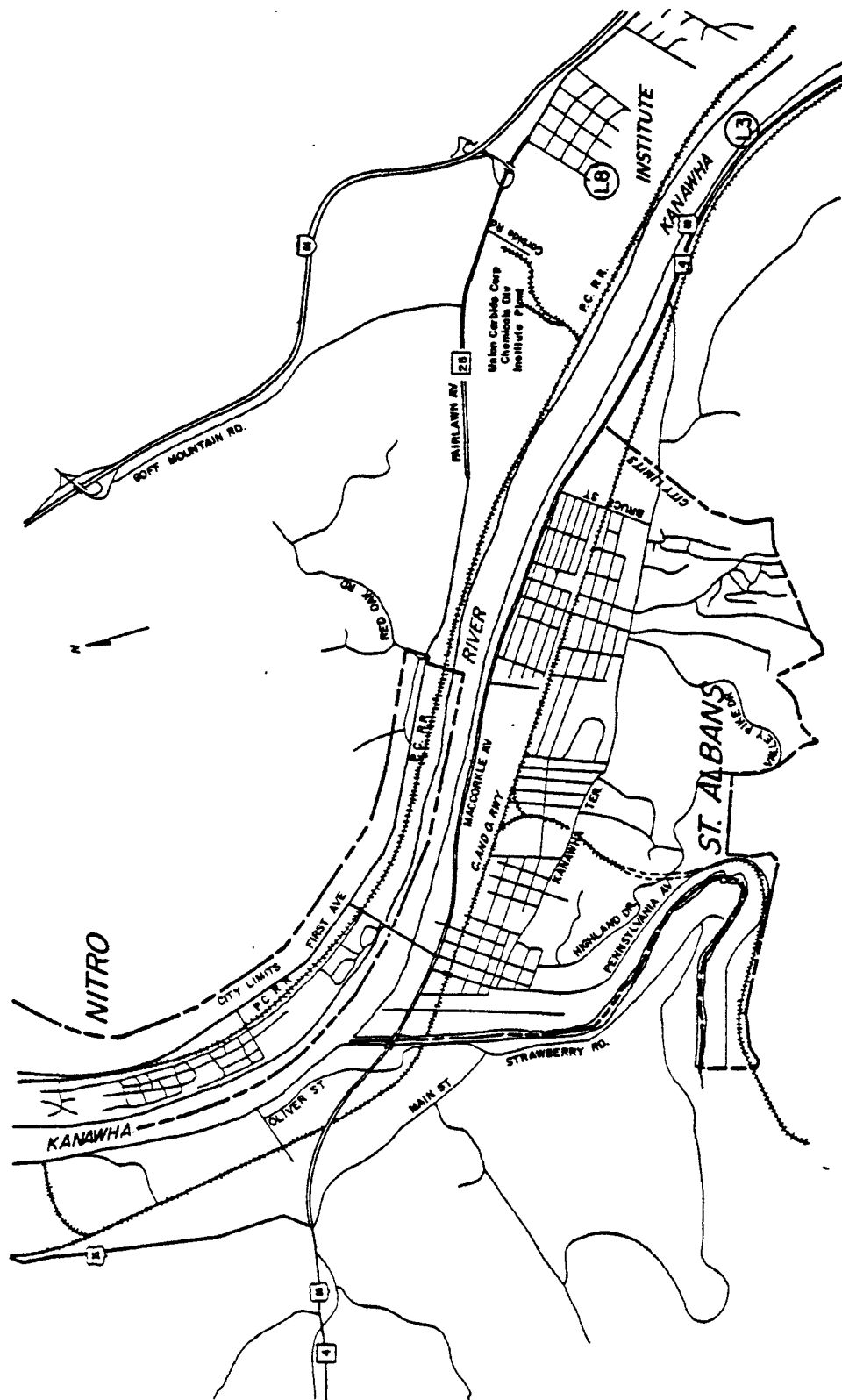


Figure 4. Map of area around St. Albans and Institute, WV showing L3 and L8 (See Table 1).

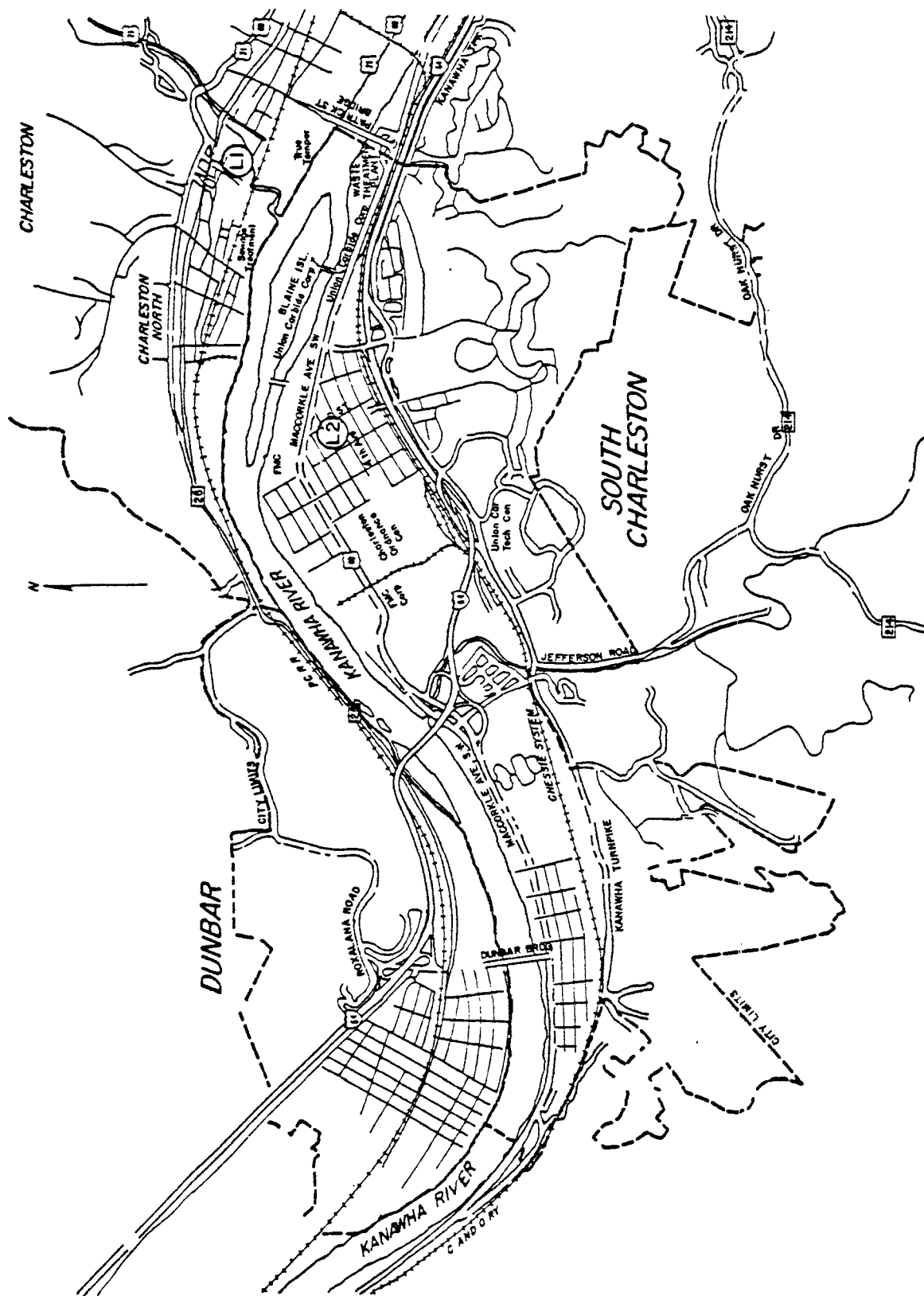


Figure 5. Map of area around Charleston and South Charleston, WV showing L1 and L2 •
(See Table 1).

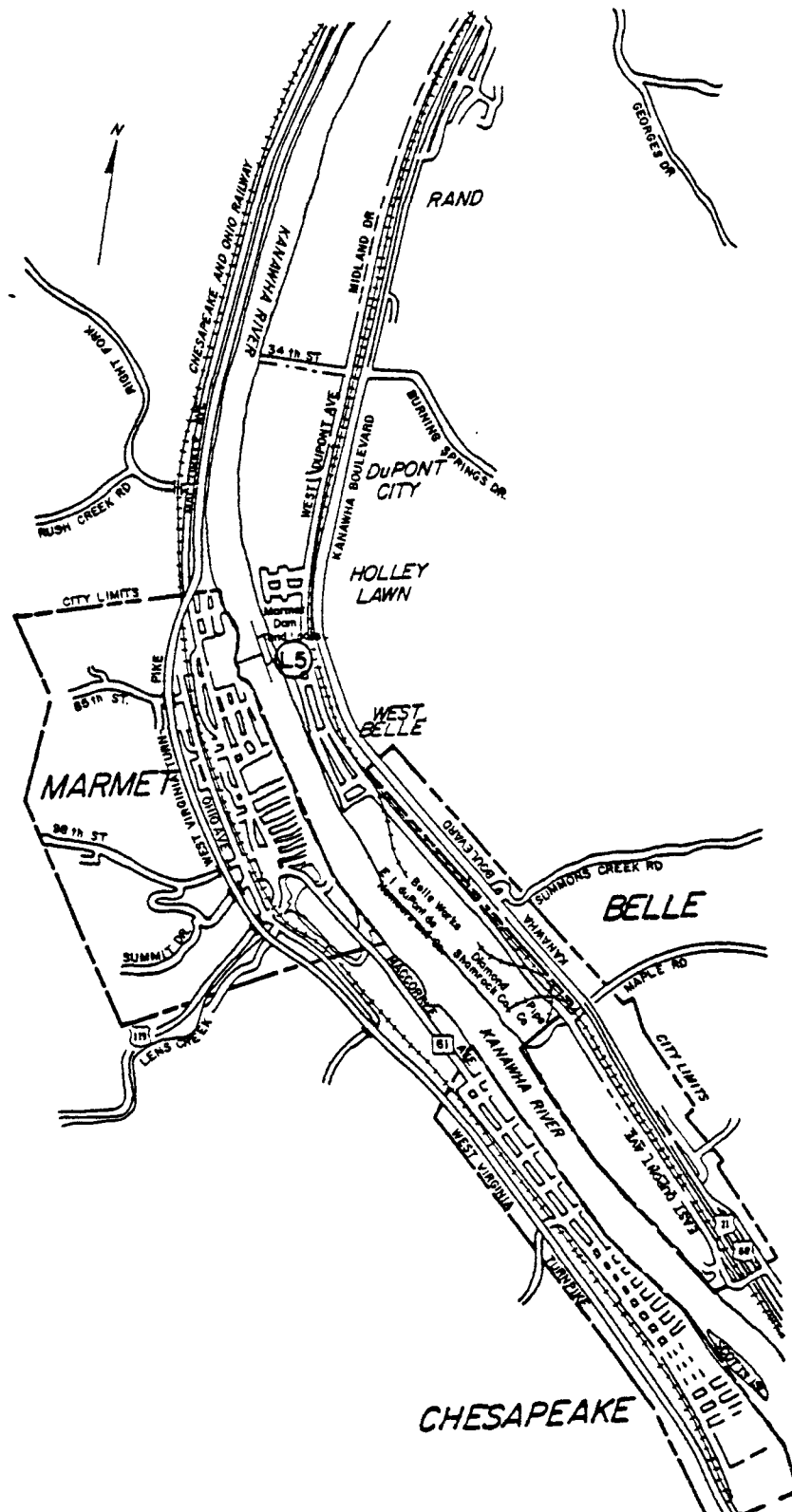


Figure 6. Map of area around W. Belle, WV showing L5 (See Table 1).

Shenandoah Valley

The Shenandoah Valley, near Front Royal, Virginia, is less highly industrialized than the Kanawha Valley. However, the potential for man-made pollution above and beyond that of day-to-day human activity does exist. In Front Royal, Allied Chemical Corporation operates an organic chemicals plant and Avtex, Inc. produces cellulosic man-made fibers. The other manufacturers listed⁽¹²⁾ in Front Royal and the small towns in the vicinity include fabric mills, clothing manufacturers, canneries, producers of crushed rock, and printers. Because of its size (2200 employees), the Avtex plant may be assumed to be the primary industrial source of organic compounds in ambient air.

The rationale for selection of sampling locations in the Shenandoah Valley, VA was completely different from that in the Kanawha Valley, WV. The only large industrial area of interest to this study (by direction of the project officer) was in Front Royal, where Avtex fibers and Allied Chemical Co. are located on adjoining plant sites. Since the sampling area was relatively small (Figure 7) and organic pollutants of interest were suspected of coming from a point source, sampling locations were chosen in a general array surrounding this point source. During each sampling period, locations were selected generally downwind (as determined by smell and the direction of stack emission plumes) and upwind for control. As with the Kanawha Valley, personnel determined sampling locations based on estimates of where high concentrations of pollutants might be detected, potential for human exposure, security of personnel and equipment, and other factors as necessary.

The MAS, duPont sampler, and MRI weather stations were located in downtown Front Royal at the fire department. With personnel on duty full time, this represented the safest location available in the area which also fulfilled the power requirements of the MAS. The duPont sampler and the MRI weather station were placed atop the fire station (about 10 m elevation).

The sampling locations, times, volumes, and meteorology are summarized in Tables 5-8. The location numbers in Tables 5-8 are shown on a detailed map (Figure 8).

Table 5. SAMPLING LOCATIONS IN THE SHENANDOAH VALLEY, VA.

Location	Site	Address	Remarks
L1	Front Royal	8th St. and Crosby Rd.	Press box at Bing Crosby Stadium.
L2	Front Royal	3rd St. and Villa Ave.	West side of tennis courts at Randolph Macon Academy.
L3	Front Royal	501 Grand Ave.	Back yard of private residence.
L4	Front Royal	Commerce Ave. between 4th St. and 5th St.	Front Royal Volunteer Fire Dept. MAS located on north parking lot. MRI and duPont personal sampler located on roof.
L5	Front Royal	Commerce Ave. and John Marshall Hwy.	Behind Quality Inn Motel.
L6	Front Royal	13th St. and Commonwealth Ave.	South side of tennis courts.
L7	Front Royal	13th St. and Commonwealth Ave.	Commonwealth Ave. playground.
L8	Front Royal	346 10th St.	Back yard of private residence.
L9	Front Royal	1040 Adams Ave.	Garden along S. side of private residence.

Table 6. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR
IN SHENANDOAH VALLEY, VA ---- TRIP 1

Site	Period/Location	Sampling Time	Sampling Volume (L)	Remarks [*]
Front Royal	P1/L1	1040-1655	714	At 1040, T ^a = 21°C, RH ^b = 51%. Sky clear. No odor.
Front Royal	P1/L2	1115-1715	336	At 1115, T = 21°C, RH = 40%. Sky clear. No odor.
Front Royal	P1/L3	1140-1728	657	At 1140, T = 22°C, RH = 42%. Sky clear. Noticeable and unpleasant odor. Winds: S.W. at 1140.
Front Royal	P1/L4	1550-1345 (9/29 - 9/30)	22,900,000 ^c	T = 6°C to 23°C. Wind: variable/calm to 1.7 m/s
Front Royal	P1/L4	1609-1305 (9/29 - 9/30)	228 ^d	T = 6°C to 23°C. Wind: variable/calm to 1.7 m/s no clouds. Some odor.
Front Royal	P2/L3 ^e	1735-0715 (9/29 - 9/30)	751 ^f	T = 16°C to 19°C. Wind: variable; mostly S.W./calm to 1.4 m/s.
Front Royal	P2/L5 ^e	2030-0635 (9/29 - 9/30)	567	T = 11°C to 6°C. Wind: variable/calm to 1.3 m/s. scattered clouds.
Front Royal	P3/L2	0737-1315	457	T = 12°C, RH = 82% at 0734. Sky clear. Heavy emissions and haze over Avtex.
Front Royal	P3/L3	0720-1300	576	T = 27°C, RH = 72% at 1305. Clear to partly cloudy.
Front Royal	P3/L6	0800-1325	325	T = 7°C to 20°C. Wind: variable/0.6 to 1.7 m/s. Faint odor.

^aTemperature

^bRelative humidity

^cSample collected with MAS

^dLong-term sample collected with duPont personal sampling pump.

^ePeriod 4 was an overnight sampling at two locations to sample potential nighttime emissions and/or settling due to atmospheric inversion.

^fPump malfunction during sampling period.

^{*} General weather conditions for 9/29 and 9/30: Warm, skies clear to scattered clouds. No precipitation, slight winds.

Dates: 9/29-30/77

Table 7. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR
IN SHENANDOAH VALLEY, VA --- Trip 2

Site	Period/Location	Sampling Time	Sampling Volume (L)	Remarks
Front Royal	P1/L1	1508-2150	397	At 1510, T ^a = 19°C, RH ^b = 95%, overcast, no odor. Wind: N.N.W. to variable/0.8 m/s to calm. T = 19°C ^c , RH = 87% to 90% ^c .
Front Royal	P1/L2	1455-2115	411	At 1605, T = 20°C, RH = 85%, low ceiling, light drizzle. Slight odor. Wind: N.N.W. to variable/0.8 m/s to calm.
Front Royal	P1/L3	1520-2120	474	At 1600, T = 20°C, RH = 85%, low ceiling. Mild odor. Wind: N.N.W. to variable/0.8 m/s to calm.
Front Royal	P1/L4	1550-0850 (10/27-10/28)	183 ^c	At 1550, T = 19°C, RH = 90%, overcast. No odor. Wind: N.N.W. to S.S.W./calm to 1.0 m/s.
Front Royal	P1/L5	1925-2315	457	Wind: variable/calm. T = 19 to 18°C ^c , RH = 87% to 90% ^c .
Front Royal	P2/L1	2155-0520	383 ^d	Wind: variable to S.S.W./calm to 1 m/s. T = 19 to 17°C ^c , RH = 87% to 90% ^e .
Front Royal	P2/L2	2115-0555	666	Wind: variable to S.S.W./calm to 1 m/s. At 0555, strong odor. T = 19 to 16°C ^e , RH = 87% to 90% ^e .
Front Royal	P2/L3	2126-0620	705	Wind: variable to S.W.W./calm to 1 m/s. At 0620, no odor noticeable. T = 19 to 16°C ^e , RH = 87% to 93% ^e .
Front Royal	P2/L5	2330-0645	854	Wind: variable to S.S.W./calm to 1 m/s. Much auto exhaust, diesel fumes. T = 19 to 15°C ^c , RH = 87% to 91% ^c .

^aTemperature

^bRelative humidity

^cLong-term sample collected with duPont personal sampling pump.

^dPump malfunctioned during sampling period.

^eData from National Weather Service Office, Dulles International Airport, Washington, DC.

* General weather conditions for 10/27 and 10/28: Moderate temperatures with high relative humidities after several days of steady rain.
Winds generally calm with skies overcast and low cloud cover.

Dates: 10/27-28/77.

Table 8. SAMPLING PROTOCOL FOR ORGANIC COMPOUNDS IN AMBIENT AIR
IN SHENANDOAH VALLEY, VA --- TRIP 3

Site	Period/Location	Sampling Time	Sampling Volume (L)	Remarks *
Front Royal	P1/L2	1540-2315	814	At 1545, T ^a = 8°C, RH ^b = 59%, wind: N/E ^c 2 ms.
Front Royal	P1/L4	1330-0925 (11/14-11/16)	46,300,000 ^c	T ^a = 4 to 15°C ^e , RH ^b = 37% to 82% ^e , winds: E.S.E. to S.S.W./calm to 7 m/s.
Front Royal	P1/L4	1315-0845 (11/14-11/16)	470 ^d	At 0845 (11-16), scattered clouds, no odor. Winds: S.S.W. to E.S.E./calm to 7 m/s ^e . T ^a = -4 to 15°C, RH ^b = 37% to 82% ^e .
Front Royal	P1/L7	1605-2330	1037	At 1600, strong odor apparently from Avtex. At 2330, wind calm, no odor. Winds: S.W.W. to S.S.E./ 2 to 3 m/s ^e . T ^a = 7 to 5°C, RH = 37% to 60% ^e .
Front Royal	P1/L8	1637-2335	639	At 2335, wind calm, no odor. Winds: S.S.W. to S.S.E./ 2 to 3 m/s ^e . T ^a = 7 to 5°C, RH = 37% to 60% ^e .
Front Royal	P1/L9	1700-2345	731	At 1700, slight odor. At 2345, no odor. Winds: S.S.W. to S.S.E./ 2 to 3 m/s ^e . T ^a = 7 to 5°C, RH = 37% to 60% ^e .
Front Royal	P2/L2	1000-1722	535	At 1000, overcast, no odor. T ^a = 6 to 14°C ^e , RH = 56% to 42% ^e , Winds: S. to S.S.W. /3 to 4 m/s.
Front Royal	P2/L7	1047-1705	1125	At 1047, slight odor. At 1705, no odor. T ^a = 6 to 14°C ^e RH = 56% to 42% ^e . Winds: S. to S.S.W. /3 to 4 m/s ^e .
Front Royal	P2/L8	1015-1715	478	At 1015, overcast, strong odor. T ^a = 6 to 14°C ^e , RH = 56% to 42% ^e . Winds: S. to S.S.W. /3 to 4 m/s ^e .
Front Royal	P2/L9	1030-1710	1192	At 1030, odor of cooked apple. At 1710, no odor. T ^a = 6 to 14°C ^e , RH = 56% to 42% ^e . Winds: S. to S.S.W. / 3 to 4 m/s.

^aTemperature.

^bRelative humidity.

^cSample collected with MAS.

^dLong-term sample collected with duPont personal sampling pump.

^eData from National Weather Service Office, Dulles International Airport, Washington, DC.

* General weather conditions for 11/14 through 11/16: Cool with clear to partly cloudy skies. Winds calm to brisk with occasional gusts.

Dates: 11/14-16/77.

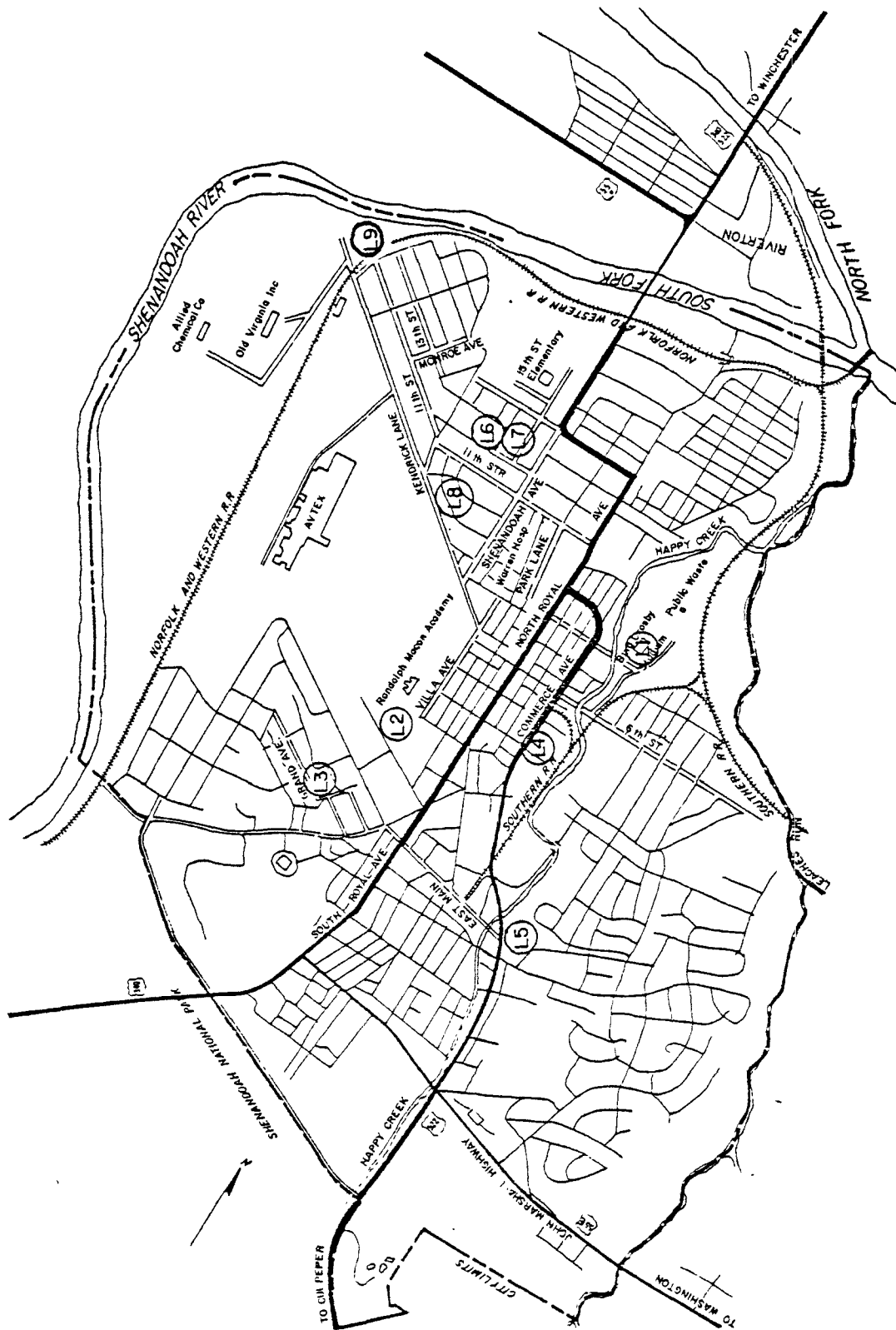


Figure 8. Map of Front Royal, VA showing sampling locations described in Table 5.

PARTICULATE COLLECTED WITH MAS

Table 9 summarizes the amounts of particulate scraped from the collection plates of the MAS. During the first trip to both locations the ionizing wires were broken and the collection of $< 1.7 \mu$ particulate was very poor. The second trip to Charleston resulted in low collection due to high humidity and occasional rain which forced operation of the sampler at a lower plate voltage (and concomitant lower collection efficiency). In addition, the rain scrubbed most of the particulate of interest out of the air. No particulate was collected on the second trip to Front Royal due to a steady rain throughout most of the sampling period. The rain not only scrubbed most of the particulate of interest from the air but also prevented operation of the MAS with any voltage supplied to the electrostatic precipitator plates due to excessive arcing. During the third trip to both Front Royal and Charleston, cool, dry weather permitted long collection periods at high plate voltages. These conditions allowed collection of more than one gram of $< 1.7 \mu$ particulate from both locations. Only the samples from Trip 3 were sufficient for GC/MS/COMP analysis.

Table 9. SUMMARY OF PARTICULATE SAMPLING WITH MAS FOR SHENANDOAH
AND KANAWHA VALLEYS

Site	Trip No.	Volume of Air Sampled (ℓ)	Amount Collected (g)		
			> 3.5 μ	3.5 - 1.7 μ	< 1.7 μ
Charleston (P1/L1)	1	29,500,000	0.1587	0.0838	0.0035 ^a
Charleston (P1/L1)	2	49,700,000	0.1653	0.1833	0.6364
Charleston (P1/L1)	3	90,800,000	0.2100	0.1552	1.8171
Front Royal (P1/L4)	1	22,900,000	0.0710	0.0391	0.2589 ^a
Front Royal (P1/L4)	2	^b	—	—	—
Front Royal (P1/L4)	3	46,300,000	0.0998	0.0558	1.1457

^a Ionizing wires were not properly charged; therefore, the amounts collected were very low.

^b No sample collected due to continuous rain and high humidity.

SECTION 6

SAMPLE ANALYSIS

ANALYSIS OF TENAX GC CARTRIDGES BY GC/MS/COMP

Air samples collected on Tenax GC cartridges were analyzed by capillary column GC/MS/COMP. The whole sample was introduced to the analytical system by thermal desorption into a cryogenic capillary trap and thence rapidly swept onto the chromatographic column. Each cartridge was loaded with a known amount of perfluorobenzene and perfluorotoluene for use in quantitation. Qualitative data interpretation was done by visual interpretation of the spectra and comparison with standard reference spectra. Quantitation was achieved by integration of a characteristic mass for a compound over the chromatographic peak. The amount of compound in the sample was then calculated using the relative molar response factor and the integrated area for a standard. The concentration in ambient air was then calculated using the volume sampled or the breakthrough volume, whichever was larger. Complete details of the sample analysis are in Appendix A.

ANALYSIS OF CARBON CARTRIDGES BY GC/MS/COMP

Carbon backup cartridges contained the very volatile compounds which have very low breakthrough volumes on Tenax GC (and thus would have high detection limits). The cartridges were not amenable to direct thermal desorption/analysis due to high background (notably water). However, the compounds of interest (methylene chloride, vinyl chloride, acetaldehyde, etc.) were eluted from the carbon cartridge at 270° onto a Tenax GC cartridge using helium. These Tenax GC transfer cartridges were then analyzed in the manner described for the Tenax GC cartridges collected in the field. This procedure was fully validated on previous contracts. Complete details of the sample analysis are in Appendix B.

ANALYSIS OF SEMIVOLATILE ORGANICS COLLECTED BY MAS SAMPLER

Extraction/Partition Scheme

Two extraction/partition schemes were used for extraction of the semivolatile organics from air particulate. The first scheme, used on the $< 1.7 \mu$ fraction collected in Charleston, WV during Trip 3, yielded six fractions. This extent of fractionation resulted in concentrations which were too low for effective GC/MS/COMP analysis. A second scheme, employed for the $< 1.7 \mu$ fraction for Front Royal, VA during Trip 3, resulted in two fractions and yielded much more concentrated samples. The GC/MS/COMP data from this sample were easier to interpret.

Analysis efforts were directed toward the $< 1.7 \mu$ fraction, as this size particle is the most easily lodged in the respiratory system and is therefore most significant with respect to potential human health effects. For reasons discussed in the Sampling Section, only the samples collected on Trip 3 were of sufficient volume to warrant extraction and analysis.

The $< 1.7 \mu$ fraction, scraped from the electrostatic precipitator plate of the MAS, was extracted by repeated sonication with cyclohexane and then with methanol. The methanol was effective in removing the more polar compounds. The extracts were then combined and fractionated according to the scheme presented in Figure 9. The individual fractions were then concentrated for GC/MS/COMP analysis. This extraction scheme was developed under another contract.⁽¹³⁾

The efficacy of the scheme was assessed by subjecting a mixture containing known amounts of compounds to the partition procedure. The mixture consisted of benzoic acid, phenol, quinoline, hexadecane, phenanthrene and ethylene glycol. The compounds were chosen to represent the five classes of materials produced by the partition scheme (all these materials have been found in air particulate samples, except ethylene glycol). No information on the composition of the polar neutral fraction was available, therefore ethylene glycol was included as a likely component of this fraction based on its known chemical properties. The experiment was conducted using both large and small mass samples. Recoveries were determined gravimetrically.

As a further check on the procedure, thin layer chromatography (TLC) scans were conducted on each fraction to ascertain the extent, if any, of

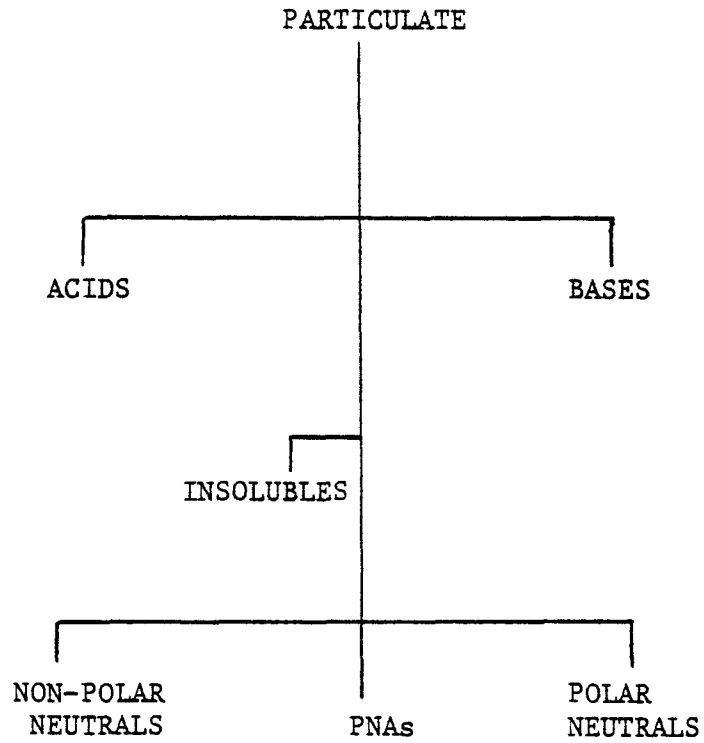


Figure 9. Fractionation scheme used for fractionating air particulate collected in Charleston, WV (Trip 3, P1/L1).

compound spillover into other fraction(s). No such spillover was detected.

Scheme Used for Front Royal, VA Sample --

The sample was weighed, 102 μg d_{10} -pyrene (Merck & Co., Rahway, NY) added as an internal standard, and allowed to equilibrate overnight. The sample was then extracted with toluene and methanol as shown in Figure 10. The two fractions thus generated were analyzed by GC/MS/COMP.

GC/MS/COMP Analysis

Samples were analyzed using a LKB 2091 gas chromatograph/mass spectrometer with a dedicated PDP-11/34 data system. The samples were chromatographed on an OV-101 capillary column (25 m, WCOT, obtained from LKB). The column was held at 100°C for 2 minutes after injection, and then heated to 265°C at a rate of 8°/min. Carrier gas flow rate was 2.0 ml/min with a split ratio of 10:1. Injector temperature was 240°C. Mass spectral scans were taken every 3 sec scanning from 5-492 amu. The ion source temperature was 200°; electron energy, 70 eV; trap current, 50 μA ; accelerating voltage 3500 V; and multiplier setting 425-450. Total ion current and mass spectra plots were generated for interpretation.

Data were interpreted by comparison of the unknown spectra with standard reference collections. Where no reference spectrum was available, or where spectral quality was not sufficient for positive identification, the compounds were labeled "tentative." All interpretations were made independently by two chemists and then correlated. Further validation of equivocal identifications was made by consultation with other chemists and spectroscopists experienced in similar research. This mass spectral interpretation protocol was established to extract the maximum information from the data and to guard against misidentification. Quantitation of the compounds identified in the semivolatile fractions was not feasible due to a lack of available standards to generate relative molar response factors. Rough quantitation may be made by comparison of peak heights on the total ion current chromatograms.

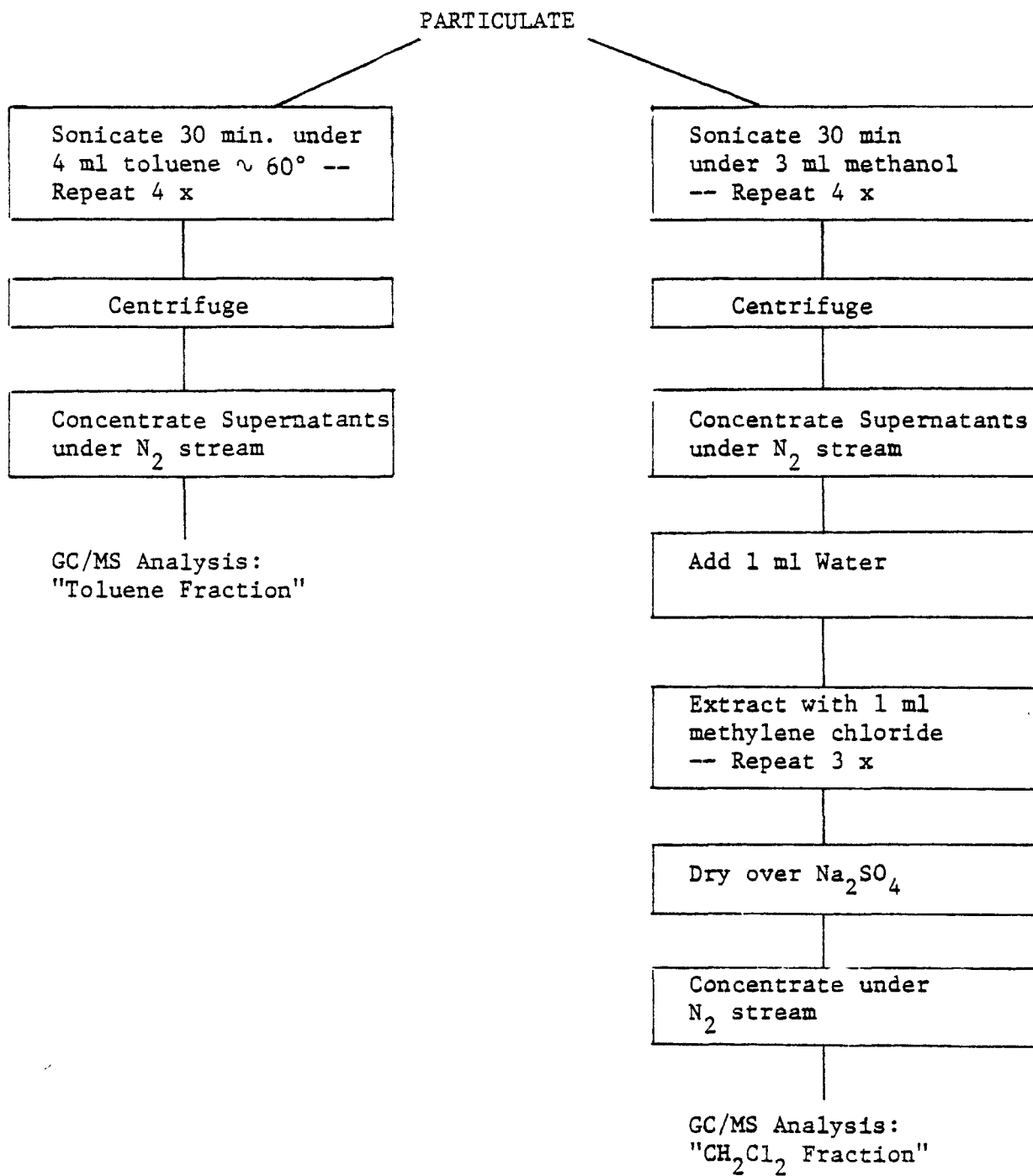


Figure 10. Extraction scheme used for fractionating air particulate collected in Front Royal, VA.

SECTION 7

RESULTS

All of the samples were analyzed for volatile and very volatile compounds. The GC/MS/COMP data were stored on magnetic tape for subsequent processing as discussed below.

Data from about one-quarter of the sampling locations were selected for qualitative interpretation. The selection of samples was based on knowledge obtained during sampling (e.g. meteorology, odor, observation of plumes, etc.) and inspection of the total ion current chromatogram from the GC/MS/COMP analysis. Only selected samples were interpreted because the compounds found in the area are not likely to be unique to a particular sample. Thus, interpretation of all data would have been redundant.

A number of compounds were selected for quantitation from the lists of compounds identified. Quantitation was performed on all samples. All halogenated compounds found were quantitated and only representative compounds from other classes were quantitated. The values presented in the tables below were not corrected for recoveries. The recoveries of standards loaded onto cartridges are presented in Table 11. Since recovery corrections were not made, all concentrations must be regarded as minima. Where trace (not quantitated) levels were observed, the designation "T" is followed by the detection limit in parentheses. Where no compound was observed, the detection limit is shown. The detection limits varied widely and were dependent upon the breakthrough volume (which is temperature-dependent), volume sampled, and relative molar response, as discussed above. As these parameters were not constant among the samples, the detection limits varied widely. In some cases compounds were identified in the qualitative analysis scheme, but were reported below the detection limit in the quantitation. This is due to the threshold set during the quantitation to prevent noise from being quantitated and reported. Thus, trace quantities which were observed in the qualitative data interpretation were not detected during quantitation. These samples may be regarded as trace.

Table 10. RECOVERIES OF SELECTED ORGANIC VAPORS FROM TENAX CARTRIDGES SUBJECTED TO
SAMPLE TRANSPORTATION AND STORAGE

Trip No.	Chemical	Quantity Added (ng)	Quantity Observed (ng)	% Recovery
1	methylene chloride	325	260	80
	chloroform	197	108	55
	1,1,1-trichloroethane	35	24	69
	benzene	249	234	93
	toluene	112	117	104
2	methylene chloride	300	218	72
	chloroform	200	109	55
	1,1,1-trichloroethane	35	20	57
	benzene	241	268	111
	toluene	110	77	70

ORGANIC COMPOUNDS IN THE KANAWHA VALLEY, WV

Volatile Organics

The volatile compounds identified on Tenax GC and/or carbon cartridges at ten locations are presented in Table 11. Alkanes and alkenes were generally not listed in the summary tables due to their ubiquity and relatively benign environmental effects. Full lists of the compounds found in each sample are contained in Appendix C. The quantitative results for the halogenated hydrocarbons and representative compounds in other chemical classes are presented in Tables 12-14 and 15-17, respectively.

Halogenated Hydrocarbons--

The levels of halogenated hydrocarbons in the Kanawha Valley during the first trip were generally low. Significantly higher levels were observed on the second trip, especially in South Charleston (P2/L2). During the third trip, significant levels of some compounds were observed at several sites, including S. Charleston (P3/L2) Charleston (P1/L1), and Institute (P2/L8).

Trichloroethylene concentrations at L4 were consistently higher than at other locations. Similarly, higher concentrations of tetrachlorethylene were observed occasionally in South Charleston (L2). High levels of chloroform, methylene chloride, and carbon tetrachloride did not seem to be correlated to any specific location and were often independent of each other.

Volatile Organics - (Non-halogenated)--

As with the halogenated compounds, the organic concentrations during the first trip were generally low. Very high concentrations were observed during the second trip in St. Albans and, to a lesser extent in S. Charleston. Moderately high levels of some compounds were observed in Institute during both sampling periods of Trip 3.

As expected, the levels of aromatics (benzene, toluene, and naphthalene) show a loose general correlation. The acetophenone level on Trip 3, P2/L2 was more than ten times higher than any other observed level. Similarly, the ethyl acetate level on Trip 2, P2/L3 was 30 times higher than in any other sample.

Table 11. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
<u>HALOGENATED</u>										
Vinylidene chloride and/or dichloro- ethylene isomer	T ^d	+	+	-	-	+	+	+	+	+
Methylene chloride	+	+	+	+	+	+	+	+	+	+
Chloroform	+	+	+	+	+	+	+	+	+	+
1,2-Dichloroethane	T	-	-	T	-	-	-	-	-	-
1,1,1-Trichloroethane	+	+	+	+	+	-	+	+	+	-
1-Chlorobutane	-	-	-	-	+	-	-	-	-	-
Carbon tetrachloride	+	+	-	+	+	+	+	+	+	-
Dichloropropene	-	-	-	-	+	-	-	-	-	-
Trichloroethylene	+	T	T	+	+	-	-	-	+	-
1,2-Dibromoethane	-	-	-	T	T	-	-	-	-	-
Tetrachloroethylene	+	+	+	+	+	T	+	+	+	-
Chlorobenzene	-	-	-	-	-	-	+	-	-	-
Dichlorobenzene	+	+	T	+	+	-	+	+	+	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
<u>ALDEHYDES</u>										
Acetaldehyde	+	+	+	+	T	+	+	+	+	-
2-Methylpropanal	-	-	-	+	+	-	-	-	-	-
n-Butanal	T	-	+	-	-	-	T	-	+	-
n-Pentanal	+	-	-	-	-	-	-	-	-	-
2-Ethylbutanal	-	-	-	+	-	-	-	-	-	-
n-Hexanal	-	T	-	-	-	+	-	-	+	-
Dimethylpentanal	-	-	-	-	+	-	-	-	-	-
n-Heptanal	T	-	-	+	-	+	-	-	-	-
Benzaldehyde	+	+	+	+	+	+	+	+	+	-
n-Octanal	T	+	+	-	-	+	-	-	+	-
n-Nonanal	-	+	+	-	-	+	+	+	+	-
n-Decanal	-	+	-	-	-	+	-	+	-	-
n-Undecanal	-	T	-	-	-	+	-	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location						
	Trip 1		Trip 2		Trip 3		
	P2/L2 ^a	P2/L5 ^a P2/L6 ^a	P2/L3 ^b	P2/L4 ^b P2/L5 ^b	P1/L8 ^a P2/L1 ^b P2/L2 ^b	P2/L9 ^c	
<u>KETONES</u>							
Acetone	+	+	+	+	+	+	+
Methyl isopropyl ketone	+	-	T	-	-	-	-
Methyl vinyl ketone	T	-	-	-	-	-	-
Methyl ethyl ketone	-	+	+	T	T	-	-
3-Pentanone	-	-	+	-	-	-	-
4-Methyl-2-pentanone	+	-	+	+	+	-	-
C ₆ H ₁₀ O isomer	-	-	-	-	T	-	-
C ₆ H ₁₂ O isomer	-	-	-	-	T	+	-
4-Methyl-3-penten-2-one	-	-	-	-	+	-	-
C ₇ H ₁₄ O isomer	-	-	T	-	-	-	-
Heptanone	-	-	-	-	+	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
KETONES (continued)										
C ₉ H ₁₈ O isomer	-	-	-	-	-	-	+	-	-	-
Acetophenone	+	+	+	-	-	+	+	+	T	-
3,5,5-Trimethyl-2-cyclohexenone	-	-	-	-	-	-	+	-	-	-
2-Pyrone	-	-	-	-	-	-	T	-	-	-
C ₁₀ H ₂₀ O isomer	-	-	-	-	-	-	-	+	-	-
2,6,8-Trimethyl-nonanone	-	-	-	-	-	-	+	-	-	-
C ₁₂ H ₂₄ O isomer	-	-	-	-	-	-	T	-	-	-
C ₁₀ H ₁₀ O ketone isomer	-	-	-	-	+	-	-	-	-	-
α-Tetralone	-	-	-	-	-	-	+	-	-	-
1,2,3,4-Tetrahydronaphthalene-1-one	-	-	-	-	-	-	-	-	+	-
Alkyl ketone	-	-	-	-	-	-	-	-	+	-
Benzophenone	-	-	-	-	+	-	+	+	+	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1		Trip 2				Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
<u>ESTERS</u>										
Methyl formate	-	-	-	T	-	-	-	-	-	-
Methyl acetate	-	-	-	+	+	-	T	-	-	-
Ethyl acetate	-	+	+	+	T	T	-	+	-	-
Isopropyl acetate	-	-	-	+	T	-	-	-	-	-
Isopropenyl acetate	-	-	-	+	-	-	-	-	-	-
n-Propyl acetate	-	-	-	+	+	-	-	-	-	-
n-Butyl acetate	-	-	-	+	-	-	-	-	-	+
C ₆ H ₁₁ acetate	-	-	-	+	-	-	-	-	-	-
<u>ALCOHOLS</u>										
Isopropanol	-	-	-	T	+	-	-	-	-	-
2-Hexanol	-	-	-	-	-	-	+	-	-	-
Alcohol isomer	-	-	-	T	-	-	-	-	-	-
Phenol	+	+	-	T	-	+	+	+	T	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1		Trip 2				Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
<u>ALCOHOLS (continued)</u>										
Cresol	-	-	-	-	-	+	-	-	-	-
Dimethylphenol isomer	-	-	-	-	-	+	-	-	-	-
C ₂ -alkyl phenol	+	+	T	+	+	+	-	+	-	-
C ₃ -alkyl phenol	-	+	-	-	-	+	-	-	-	-
<u>ETHERS</u>										
Dimethyl ether	-	+	+	T	-	+	+	-	-	-
Diethyl ether	-	+	+	-	-	-	-	+	T	+
Furan	T	-	-	T	-	-	-	-	T	-
Diisopropyl ether	-	-	-	+	+	+	+	-	-	-
Alkyl ether	-	-	-	T	-	-	-	-	-	-
Alkyl ether	-	-	-	-	-	-	+	-	-	-
2-Methoxy-2h-dihydro-pyran	-	-	-	-	-	-	+	-	-	-
Anisole	-	-	-	-	+	-	-	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1		Trip 2			Trip 3			
	P2/L2 ^a	P2/L5 ^a P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
ETHERS (continued)									
Benzofuran	-	-	-	-	-	+	-	-	-
Diphenyl ether	+	T	-	+	-	+	-	-	-
ARONATICS									
Benzene	+	+	+	+	+	+	+	+	-
Toluene	+	+	+	+	+	+	+	+	-
Ethylbenzene	+	+	+	+	+	+	+	+	-
Styrene	+	+	+	+	+	+	+	+	-
Xylene	+	+	+	+	+	+	+	+	-
Propylbenzene	+	+	+	+	+	+	+	+	-
Ethyltoluene	+	+	+	+	+	+	+	+	-
Trimethylbenzene	+	+	+	+	+	+	+	+	-
o-Ethyltoluene	+	+	+	+	-	+	+	+	-
C ₃ H ₅ benzene	-	-	+	+	-	-	+	+	-
C ₃ -alkylbenzene	-	-	+	-	+	-	+	-	-
Methylstyrene isomer	-	-	-	-	-	-	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1		Trip 2				Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
<u>AROMATICS (continued)</u>										
C ₄ -alkylbenzene	+	+	+	+	+	+	+	+	+	-
i-Butylbenzene	-	-	-	+	-	-	-	-	+	-
sec-Butylbenzene	-	-	-	+	-	-	-	-	+	-
Indan	+	+	+	+	+	-	+	+	-	-
Indene	-	-	-	-	-	-	+	-	-	-
n-Butylbenzene	-	-	+	-	+	-	-	-	-	-
Propyltoluene	-	-	-	+	-	-	-	-	+	-
C ₅ -alkylbenzene	+	+	+	+	+	-	+	+	+	-
Tetramethylbenzene	-	-	-	+	+	-	-	-	+	-
1,2,3,4-Tetrahydro-naphthalene	+	-	-	+	+	-	+	-	+	-
C ₄ H ₇ benzene isomer	-	+	-	+	+	-	+	+	+	-
Naphthalene	+	+	+	+	+	-	+	+	+	-
Methyldihydro-naphthalene	-	-	-	-	-	-	T	-	-	-
C ₅ H ₉ benzene isomer	+	-	-	+	-	-	-	-	+	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location									
	Trip 1			Trip 2			Trip 3			
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P1/L8 ^a	P2/L1 ^b	P2/L2 ^b	P2/L9 ^c
AROMATICS (continued)										
C ₆ -alkylbenzene	+	-	-	+	+	-	-	-	+	-
β-Methylnaphthalene	+	+	+	+	+	+	+	+	+	-
α-Methylnaphthalene	+	+	+	+	+	-	+	+	+	-
C ₆ H ₁₁ benzene	-	-	-	-	T	-	-	-	-	-
C ₇ -Alkylbenzene	-	-	-	-	+	-	-	-	-	-
C ₂ -Alkyl-naphthalene	-	T	+	+	-	-	+	+	-	-
Dimethylnaphthalene isomer	+	-	-	+	+	-	-	+	+	-
Biphenyl	+	+	-	+	+	T	+	-	+	-
C ₃ -Alkyl-naphthalene	-	-	-	+	+	-	-	-	-	-
SULFUR CONTAINING										
CS ₂	+	+	+	+	+	-	-	-	-	+
Dimethyl disulfide	-	-	-	-	+	-	-	-	-	-
2,3-Benzothioephene	-	-	-	-	-	-	T	-	-	-

(continued)

Table 11. (cont'd.)

CHEMICAL CLASS	Period/Location							
	Trip 1		Trip 2			Trip 3		
	P2/L2 ^a	P2/L5 ^a	P2/L6 ^a	P2/L3 ^b	P2/L4 ^b	P2/L5 ^b	P2/L1 ^b	P2/L2 ^b P2/L9 ^c
<u>NITROGEN CONTAINING</u>								
Cyanobenzene	-	-	-	-	-	-	-	-
C ₃ -alkyl pyridine	-	-	-	-	-	T	-	-
<u>MISCELLANEOUS</u>								
Butene	-	+	+	-	-	-	-	-
4-Vinylcyclohexene	-	-	-	-	+	-	-	-

Notes

^aBoth Tenax GC and carbon cartridge samples interpreted^bTenax GC cartridge sample interpreted^cCarbon cartridge sample interpreted^d+ = identified

- = not identified

T = tentative identification

[alkanes, alkenes, and artifacts not included]

Table 12. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR
FROM THE KANAWHA VALLEY, WV --- TRIP 1.

Chemical	Period/Location									
	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L5	P2/L6	
methylene chloride	T(1000)	T(1000)	T(714)	T(714)	<625	T(555)	778	<555	<555	
chloroform	T(167)	T(167)	T(125)	T(125)	<120	T(97)	T(97)	<97	<97	
carbon tetrachloride	<625	T(125)	<95	T(95)	<91	T(74)	T(74)	<74	<74	
vinyl chloride	<15000	<12000	<12000	<12000	<10000	<10000	<10000	<10000	<10000	
1,2-dichloroethylene	<545	<334	T(334)	<334	T(322)	<322	T(322)	<263	<263	
1,1-dichloroethane	<380	<286	<285	<285	<345	<345	<345	<228	<228	
1,2-dichloroethane	T(347)	T(258)	<258	<258	T(250)	<256	<256	<195	<195	
1,1,1-trichloroethane	T(417)	T(334)	T(334)	T(334)	T(312)	T(312)	T(312)	<278	<278	
1,1,2-trichloroethane	<294	<250	<250	<250	<238	-	<217	<218	<218	
trichloroethylene	T(132)	T(100)	<100	300	<98	T(98)	T(98)	<74	<74	
tetrachloroethylene	T(48)	T(35)	T(36)	<36	T(36)	146	T(26)	<26	<26	
1,1,1,2-tetrachloroethane	<23	<31	<31	<31	<30	<30	<30	<22	<22	
1,1,1,2,2-tetrachloroethane	<23	<31	<31	<31	<30	<30	<30	<22	<22	
pentachloroethane	<13	<8	<9	<10	<9	<9	<9	<9	<12	
hexachloroethane	<13	<8	<9	<10	<9	<9	<9	<9	<12	
chlorobenzene	<58	<25	<27	T(32)	<32	<32	<32	<27	<36	
o-dichlorobenzene	<39	T(17)	<18	<20	<18	T(18)	<18	<18	<24	
m-dichlorobenzene	<39	T(28)	T(18)	T(20)	T(18)	38	<14	<18	<24	
p-dichlorobenzene	<35	<15	<16	<18	<16	<16	-	<17	<30	
1,2,4-trichlorobenzene	<23	<10	<11	<12	<11	<11	<8	<11	<15	
1,3,5-trichlorobenzene	<13	<8	<9	<10	<9	<9	<7	<9	<12	
1,2,3-trichlorobenzene	<23	<10	<11	<12	<11	<11	<8	<11	<15	
vinylidene chloride	<454	<334	<334	<334	<345	<345	<345	<263	<263	

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceded by <.

Table 13. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR
FROM THE KANAWHA VALLEY, WV --- TRIP 2.

Chemical	Period/Location											
	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L4	P2/L5	B		
methylene chloride	867	715	T(714)	T(714)	T(714)	11334	T(555)	T(555)	1778	<7		
chloroform	177	T(125)	T(125)	T(125)	T(125)	2161	161	1333	T(97)	<3		
carbon tetrachloride	215	T(95)	T(95)	T(95)	T(95)	2222	3630	97	T(74)	<2		
vinyl chloride	<10000	<12000	<12000	<12000	<12000	<10000	<10000	<10000	<10000	<15		
1,2-dichloroethylene	T(263)	<334	<334	T(334)	T(334)	T(263)	<263	<263	T(263)	<10		
1,1-dichloroethane	<228	<228	<228	<228	<228	<228	<228	<228	<228	<8		
1,2-dichloroethane	T(195)	T(258)	<258	T(258)	<258	T(195)	T(195)	T(195)	T(195)	<8		
1,1,1-trichloroethane	278	T(334)	T(334)	T(334)	T(334)	3278	T(278)	T(278)	<278	<5		
1,1,2-trichloroethane	<217	<250	<250	<250	<250	<217	<217	<217	<217	<5		
trichloroethylene	<74	<100	<100	360	T(100)	179	45	358	T(75)	<5		
tetrachloroethylene	109	T(36)	<36	T(360)	T(36)	1536	434	52	<26	<7		
1,1,1,2-tetrachloroethane	<22	<31	<31	<31	<31	<20	<22	<22	<22	<6		
1,1,2,2-tetrachloroethane	<22	<31	<31	<31	<31	<20	<22	<22	<22	<6		
pentachloroethane	<10	<19	<13	<13	<12	<17	<12	<12	<9	<5		
hexachloroethane	<10	<19	<13	<13	<12	<17	<12	<12	<9	<5		
chlorobenzene	T(29)	T(56)	<40	<40	T(36)	44	<35	T(37)	<26	<15		
o-dichlorobenzene	<19	T(37)	<27	T(27)	<24	306	T(23)	39	<17	<10		
m-dichlorobenzene	101	T(37)	<27	T(27)	T(24)	276	T(23)	T(24)	<17	<10		
p-dichlorobenzene	<18	<34	<24	<24	<22	T(33)	<21	<22	<16	<9		
1,2,4-trichlorobenzene	<12	<22	<16	<16	<14	<20	<14	<15	<12	<6		
1,3,5-trichlorobenzene	<10	<19	<13	<13	<12	<17	<12	<12	<9	<5		
1,2,3-trichlorobenzene	<12	<22	<16	<16	<14	<20	<14	<15	<12	<6		
vinylidene chloride	T(263)	<334	<334	<334	<334	<263	<263	<263	<263	<10		

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceded by <.

Table 14. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR
FROM THE KANAWHA VALLEY, WV ---- TRIP 3

Chemical	Period/Location											
	P1/L1	P2/L2	P2/L5	P2/L7	P2/L8	P3/L1	P3/L2	P3/L5	P3/L8	P3/L9		
methylene chloride	2818	T(454)	T(454)	T(454)	4091	1636	9818	1272	1636	1600		
chloroform	428	T(71)	T(71)	T(71)	333	T(71)	262	T(71)	T(71)	T(71)		
carbon tetrachloride	529	T(59)	T(59)	T(59)	441	T(59)	500	T(59)	T(59)	T(59)		
vinyl chloride	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500		
1,2-dichloroethylene	T(212)	T(213)	T(212)	T(213)	T(213)	T(213)	T(213)	<213	<213	T(213)		
1,1-dichloroethane	<160	<160	<160	<160	<160	<160	<160	<160	<160	<160		
1,2-dichloroethane	T(151)	151	T(163)	T(151)	T(151)	T(151)	T(151)	T(151)	T(151)	T(151)		
1,1,1-trichloroethane	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	347	T(217)		
1,1,2-trichloroethane	<167	<167	<94	<167	<167	<167	<167	<167	<167	<167		
trichloroethylene	T(56)	T(56)	T(55)	T(55)	T(55)	T(55)	T(55)	T(55)	T(55)	<144		
tetrachloroethylene	T(20)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)		
pentachloroethane	<14	<6	<6	<6	<6	<6	<6	<6	<6	<6		
hexachloroethane	<14	<6	<6	<6	<6	<6	<6	<6	<6	<6		
chlorobenzene	<44	<17	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)		
o-dichlorobenzene	<29	<9	T(8)	T(12)	59	<9	T(9)	T(9)	T(9)	T(9)		
m-dichlorobenzene	<29	<16	T(8)	T(12)	T(12)	<18	<9	T(9)	T(9)	T(9)		
p-dichlorobenzene	<26	<8	<7	<7	<7	<7	<7	<7	<7	<7		
1,2,4-trichlorobenzene	<17	<6	<7	<7	<7	<7	<7	<7	<7	<7		
1,3,5-trichlorobenzene	<14	<6	<6	<6	<6	<6	<6	<6	<6	<6		
1,2,3-trichlorobenzene	<17	<6	<7	<7	<7	<7	<7	<7	<7	<7		
vinylidene chloride	<212	<213	<212	<213	<213	<213	<213	<213	<213	<213		
1,1,1,2-tetrachloroethane	<17	<16	<17	<16	<16	<16	<16	<16	<16	<16		
1,1,2,2-tetrachloroethane	<17	<16	<17	<16	<16	<16	<16	<16	<16	<16		

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceded by <.

Table 15. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM THE
KANAWHA VALLEY, WV ---- TRIP 1.

Chemical	B	Period/Location										
		P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L5	P2/L6		
benzene	<3	259	117	44	28	69	36	83	102	120		
toluene	<3	178	212	27	115	83	518	95	297	310		
naphthalene	<3	31	55	9	17	13	57	8	24	32		
acetophenone	<10	T(39)	80	<18	78	41	217	<14	54	124		
n-octanal	<10	T(39)	11	18	T(20)	T(18)	T(22)	T(18)	T(2)	T(30)		
benzophenone	<10	T(39)	T(17)	T(18)	T(20)	T(18)	T(18)	T(14)	<18	<24		
phenol	<15	T(58)	16	20	T(30)	13	T(27)	<21	13	T(37)		
diphenyl ether	<10	<39	<17	T(18)	T(20)	<18	<18	<14	T(18)	<24		
ethyl acetate	<7	<43	T(43)	<43	<43	<43	T(97)	T(31)	<43	T(43)		
cyanobenzene	<5	T(15)	10	6	T(10)	<9	20	<7	<9	<12		
dimethyldisulfide	<8	<77	<77	<77	68	<77	163	<77	<77	<77		

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceeded by <.

B = blank control. Values are in ng/cartridge.

Table 16. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM THE
KANAWHA VALLEY, WV ---TRIP 2

	Period/Location									
	P1/L6	P1/L2	P1/L3	P1/L4	P1/L5	P2/L2	P2/L3	P2/L4	P2/L5	B
benzene	1611	259	203	185	389	3444	71778	296	593	<3
toluene	1441	93	144	241	192	1297	2865	906	392	<3
naphthalene	87	T(7)	29	34	13	3758	4694	321	23	<3
acetophenone	195	173	168	740	136	4950	<23	24	91	<10
n-octanal	<29	T(22)	<22	1044	T(44)	167	<22	24	T(22)	<10
benzophenone	T(29)	48	<22	<21	<22	374	<23	T(24)	22	<10
phenol	T(44)	20	<36	32	24	415	743	36	42	<15
diphenyl ether	<29	<25	<22	<21	<22	T(34)	208	T(24)	T(18)	<10
ethyl acetate	T(43)	T(97)	<97	T(97)	T(97)	91	6917	97	208	<7
cyanobenzene	24	<12	<12	<10	11	<17	<35	<12	<8	<5
dimethyldisulfide	<77	<163	<163	<163	<163	489	489	388	<489	<8

Values in ng/m³.

T = trace, values in parentheses are detection limits.

no compound was detected, the detection limit is listed preceded by <. Blank control. Values are in ng/cartridge.

Table 17. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM THE
KANAWHA VALLEY, WV ---- TRIP 3

Chemical	Period/Location									
	P1/L1	P2/L2	P2/L5	P2/L7	P2/L8	P3/L1	P3/L2	P3/L5	P3/L8	P3/L9
benzene	334	555	305	778	2185	667	315	667	2287	250
toluene	53	449	111	<103	714	654	502	452	152	295
naphthalene	29	111	11	108	80	87	73	28	280	19
acetophenone	93	143	71	171	319	195	317	62	132	63
n-octanal	T(29)	25	T(18)	T(14)	T(18)	<29	<18	<18	14	345
benzophenone	<29	<9	<8	<21	T(12)	T(29)	46	T(9)	T(13)	10
phenol	20	8	11	38	42	T(44)	6	T(14)	10	T(15)
diphenyl ether	<29	<9	<8	<21	T(12)	<29	<16	<9	T(13)	T(10)
ethyl acetate	T(43)	T(43)	T(43)	T(43)	83	T(43)	T(43)	43	49	T(43)
cyanobenzene	T(14)	20	15	35	45	24	11	10	12	T(8)
dimethyldisulfide	<77	<77	<77	<77	<77	<77	<77	<77	<77	T(77)

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceded by <.

Correlation between Levels of Halogenated and Non-halogenated Organics --

There are no general correlation between the levels of halogenated and non-halogenated organics in the Kanawha Valley. Two samples (Trip 2, P2/L2 and P2/L3) contained high levels of both halogenated and non-halogenated compounds.

Semivolatiles

The compounds identified in the polar neutral, PNA, paraffin and base fractions of the $<1.7 \mu$ air particulate are shown in Appendix D. The few compounds identified in the acid fraction were contained in other fractions also. It should be noted that the computer scales the TIC plot to the largest peaks. Therefore quantitative comparisons between fractions are not possible.

ORGANIC COMPOUNDS IN THE SHENANDOAH VALLEY, VA

Volatile Organics

A summary of the volatile compounds identified on Tenax GC and/or carbon cartridges at nine locations are presented in Table 18. Alkanes and alkenes were generally not summarized because of their ubiquity and relatively benign environmental effects. Full lists of the compounds found in each sample are contained in Appendix E. The quantitation results for the halogenated hydrocarbons and representative compounds in other chemical classes are presented in Tables 19-21 and 22-24, respectively.

The highest concentrations of volatile organics found on Trip 1 was at P2/L3 and P2/L5 which were night samples. P2/L3 was downwind of the Avtex plant at least part of the sampling period. The other samples obtained on this trip contained moderate amounts of volatile organics. The samples collected during Trip 2 contained high amounts of volatile compounds. The highest concentrations were again in the overnight samples (P1/L4, P2/L3, and P2/L5). L4 and L5 were in the downtown Front Royal area, which was in the floor of the valley. Thus, settling of pollutants in the lower areas during a night-time atmospheric inversion may have contributed to these high values. The other location (L3), however, was on top of a hill, so atmospheric inversion conditions would not explain high values at this point. The values obtained for P1/L3 were also relatively high. This sample was collected during the late afternoon-evening, so some of the

Table 18. VOLATILE ORGANICS IDENTIFIED IN AMBIENT AIR IN THE SHENANDOAH VALLEY, VA (FRONT ROYAL)

CHEMICAL CLASS	Period/Location						
	Trip 1			Trip 2		Trip 3	
	P1/L4 ^a	P2/L5 ^a	P3/L2 ^b	P3/L6 ^c	P2/L3 ^b	P3/L5 ^b	P1/L9 ^a P2/L8 ^b P2/L9 ^b
<u>HALOGENATED</u>							
Vinylidene chloride and/or dichloroethylene isomer	+	+	+	+	+	+	+
Methylene chloride	+	+	+	+	+	+	+
Chloroform	+	+	+	+	+	+	+
1,2-Dichloroethane	-	-	-	-	T	-	-
1,1,1-Trichloroethane	-	-	-	+	+	-	+
Carbon tetrachloride	-	-	+	T	+	+	+
Trichloroethylene	-	-	-	-	+	-	+
Tetrachloroethylene	-	-	+	+	+	+	+
Dichlorobenzene	-	-	T	+	+	-	+
<u>ALDEHYDES</u>							
Acetaldehyde	+	+	+	+	+	+	+
Propanal	-	+	-	-	-	-	-
n-Butanal	-	+	+	+	-	+	-

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1			Trip 2			Trip 3		
	P1/L4 ^a	P2/L5 ^a	P3/L2 ^b	P3/L6 ^c	P2/L3 ^b	P3/L5 ^b	P1/L9 ^a	P2/L8 ^b	P2/L9 ^b
<u>ALDEHYDES (continued)</u>									
n-Pentanal	-	+	T	+	+	-	-	+	-
n-Hexanal	-	+	+	+	-	T	-	+	-
n-Heptanal	-	-	+	+	-	-	-	+	-
Benzaldehyde	-	-	+	+	+	+	-	+	+
n-Octanal	-	-	+	+	-	+	-	T	+
n-Nonanal	-	-	+	+	+	+	-	+	+
n-Decanal	-	-	+	+	-	+	-	+	+
n-Undecanal	-	-	+	+	-	+	-	+	-
<u>KETONES</u>									
Acetone	+	+	+	+	+	+	+	+	+
Methyl isopropyl ketone	-	-	-	-	-	T	-	-	-
Methyl vinyl ketone	-	-	-	+	-	-	-	-	-
Methyl ethyl ketone	-	-	-	+	+	-	-	T	-
Acetophenone	-	-	+	+	+	+	-	+	+
Benzophenone	-	-	-	+	-	+	-	-	-

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1			Trip 2			Trip 3		
	P1/L4 ^a	P2/L5 ^a	P3/L2 ^b	P3/L6 ^c	P2/L3 ^b	P3/L5 ^b	P1/L9 ^a	P2/L8 ^b	P2/L9 ^b
<u>ESTERS</u>									
Ethyl acetate	-	-	+	-	+	+	-	T	-
<u>ALCOHOLS</u>									
Phenol	-	-	+	+	+	+	-	+	-
Cresol	-	-	+	+	+	+	-	+	-
Dimethylphenol isomer	-	-	+	+	+	+	-	-	-
C ₂ -alkyl phenol	-	-	+	+	+	+	-	+	-
C ₃ -alkyl phenol	-	-	+	+	+	+	-	+	-
C ₆ -alkyl phenol	-	-	+	+	+	-	-	-	-
<u>ETHERS</u>									
Diethyl ether	+	+	+	-	T	T	T	+	+
<u>AROMATICS</u>									
Benzene	+	+	+	+	+	+	-	+	+
Toluene	+	+	+	+	+	+	-	+	+
Ethylbenzene	-	-	+	+	+	+	-	+	+
Styrene	-	-	+	+	+	+	-	+	+
Xylene	-	-	+	+	+	+	-	+	+

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period/Location								
	Trip 1			Trip 2			Trip 3		
	P1/L4 ^a	P2/L5 ^a	P3/L2 ^b	P3/L6 ^c	P2/L3 ^b	P3/L5 ^b	P1/L9 ^a	P2/L8 ^b	P2/L9 ^b
1- or n-Propylbenzene	-	-	+	+	+	-	-	+	+
Ethyltoluene	-	-	+	+	+	+	-	+	+
Trimethylbenzene	-	-	+	+	+	+	-	+	+
o-Ethyltoluene	-	-	+	-	+	-	-	+	+
C ₃ -alkyl benzene	-	-	-	-	-	+	-	-	+
C ₄ -alkyl benzene	-	-	+	+	+	+	-	+	+
Indan	-	-	+	+	+	-	-	+	+
Tetramethylbenzene isomer	-	-	-	-	-	-	-	-	+
C ₅ -alkyl benzene	-	-	+	+	+	-	-	+	+
C ₄ ^H ₇ benzene isomer	-	-	-	+	+	-	-	-	-
Naphthalene	-	-	+	+	+	T	-	+	+
C ₆ -alkyl benzene	-	-	-	-	-	-	-	-	T
β-Methyl naphthalene	-	-	+	+	+	+	-	+	+
α-Methyl naphthalene	-	-	-	+	+	+	-	+	+
C ₂ -alkyl naphthalene	-	-	-	T	+	-	-	-	-
Biphenyl	-	-	-	+	T	-	-	-	T

(continued)

Table 18. (cont'd.)

CHEMICAL CLASS	Period Location								
	Trip 1			Trip 2			Trip 3		
	P1/L4 ^a	P2/L5 ^a	P3/L2 ^b	P3/L6 ^c	P2/L3 ^b	P3/L5 ^b	P1/L9 ^a	P2/L8 ^b	P2/L9 ^b
<u>SULFUR CONTAINING</u>									
SO ₂	-	-	-	-	-	-	-	-	+
CS ₂	+	+	-	+	+	-	+	-	+

Notes

- a) Carbon cartridges interpreted.
 b) Tenax GC cartridge interpreted.
 c) Both Tenax GC and carbon cartridges interpreted.
 d) + = identified
 - = not identified
 T = tentative identification
 [alkanes, alkenes, and artifacts not included].

Table 19. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR
FROM FRONT ROYAL, VA ---- TRIP 1

Chemical	Period/Location									
	P1/L1	P1/L2	P1/L3	P1/L4	P2/L3	P2/L5	P3/L2	P3/L6	B	
methylene chloride	1000	T(714)	1857	2143	97627	2444	4600	1000	^6	
chloroform	T(125)	125	125	208	4800	149	278	T(125)	<3	
carbon tetrachloride	<95	<95	T(95)	<95	190	T(74)	T(125)	T(95)	<2	
vinyl chloride	<12000	<12000	<12000	<12000	<11538	<10000	<15000	<12000	<15	
1,2-dichloroethylene	T(334)	<334	<334	T(500)	<357	<263	<454	<334	<10	
1,1-dichloroethane	<285	<285	<285	<285	<258	<228	<476	<285	<8	
1,2-dichloroethane	<258	<258	<258	<258	<500	<195	T(348)	<258	<8	
1,1,1-trichloroethane	T(334)	T(100)	T(334)	T(334)	381	T(278)	<667	T(334)	<5	
1,1,2-trichloroethane	<250	<334	<250	<250	<98	<217	<294	<250	<5	
trichloroethylene	<100	<100	<100	T(100)	T(98)	T(74)	T(132)	<100	<5	
tetrachloroethylene	T(36)	20	<36	T(36)	132	26	35	31	<7	
1,1,1,2-tetrachloroethane	<22	<30	<30	<30	<30	<22	<40	<30	<6	
1,1,1,2,2-tetrachloroethane	<22	<30	<30	<30	<30	<22	<40	<30	<6	
pentachloroethane	<7	<15	<8	<22	<7	<9	<9	<15	<5	
hexachloroethane	<7	<15	<8	<22	<7	<9	<9	<15	<5	
chlorobenzene	<32	<45	<32	<66	<32	T(26)	T(44)	<46	<15	
o-dichlorobenzene	<14	<30	<18	<44	T(13)	T(18)	<18	T(31)	<10	
m-dichlorobenzene	<14	T(27)	T(18)	22	8	T(18)	T(17)	T(31)	<10	
p-dichlorobenzene	<13	<27	<15	<39	<12	<16	<16	<28	<9	
1,2,4-trichlorobenzene	<8	<18	<9	<26	<8	<10	<10	<10	<6	
1,3,5-trichlorobenzene	<7	<15	<8	<22	<7	<9	<9	<15	<5	
1,2,5-trichlorobenzene	<8	<18	<9	<26	<8	<10	<10	<18	<6	
vinylidene chloride	<334	<334	<334	T(500)	2500	<263	778	<334	<10	

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is preceded by <.

B = blank control. Values are in ng/cartridge.

Table 20. ESTIMATED LEVELS OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR
FROM FRONT ROYAL, VA ---- TRIP 2

Chemical	Period/Location									
	P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L1	P2/L2	P2/L3	P2/L5	
methylene chloride	8375	40571	11428	120142	87375	25250	2625	111556	248250	
chloroform	692	792	T(125)	2708	1807	711	T(115)	2193	14517	
carbon tetrachloride	217	T(95)	T(95)	1190	T(87)	T(87)	565	889	280	
vinyl chloride	<12000	<12000	<12000	<12000	<11750	<12000	<11750	<10000	<11500	
1,2-dichloroethylene	T(312)	T(334)	T(334)	T(334)	T(312)	T(312)	T(312)	1842	2974	
1,1-dichloroethane	<267	<285	<285	<285	<267	<267	<334	<263	<242	
1,2-dichloroethane	T(242)	T(258)	T(258)	322	<242	T(242)	T(242)	<228	<205	
1,1,1-trichloroethane	T(294)	800	T(334)	2933	T(294)	T(470)	T(470)	195	T(312)	
1,1,2-trichloroethane	<227	<250	<250	<250	<227	<363	<227	2500	<238	
trichloroethylene	T(96)	T(100)	T(100)	420	<96	T(96)	T(96)	<218	T(77)	
tetrachloroethylene	380	332	36	2994	T(36)	163	35	388	77	
1,1,1,2-tetrachloroethane	<15	<30	<30	<33	<30	<16	<27	810	<22	
1,1,2,2-tetrachloroethane	<15	<30	<30	<33	<30	<16	<27	<22	<22	
pentachloroethane	<12	<12	<11	<27	<11	<13	<8	<22	<6	
hexachloroethane	<12	<12	<11	<27	<11	<13	<8	<7	<6	
chlorobenzene	T(38)	T(36)	T(32)	T(82)	<33	<39	<32	<7	<18	
o-dichlorobenzene	58	T(24)	T(21)	T(55)	<22	<26	<15	38	<12	
m-dichlorobenzene	35	T(24)	T(21)	279	<22	T(26)	<15	T(14)	<12	
p-dichlorobenzene	<23	<22	<19	<49	<20	<23	<14	68	<10	
1,2,4-trichlorobenzene	<15	<14	<13	<33	<13	<16	<9	<13	<7	
1,3,5-trichlorobenzene	<12	<12	<11	<27	<11	<13	<8	<9	<6	
1,2,5-trichlorobenzene	<15	<14	<13	<33	<13	<16	<9	<7	<7	
vinylidene chloride	<312	334	<334	<334	<312	<312	<312	<9	<27	

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceded by <.

Table 21. ESTIMATED LEVEL OF HALOGENATED ORGANIC VAPORS IN AMBIENT AIR
FROM FRONT ROYAL, VA ---- TRIP 3

Chemical	B	Period/Location											
		P1/L12	P1/L4	P1/L7	P1/L8	P1/L9	P2/L2	P2/L7	P2/L8	P2/L9			
ethylene chloride	<5	1364	T(454)	2545	<454	1091	1818	2090	6273	<454			
chloroform	<3	T(71)	<71	<71	<71	<71	<71	T(71)	119	<71			
carbon tetrachloride	<2	<59	T(59)	<59	<59	<59	T(59)	<59	T(59)	<59			
vinyl chloride	<15	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500	<7500			
1,2-dichloroethylene	<10	T(213)	T(213)	T(213)	<213	T(213)	T(213)	T(213)	T(213)	T(213)			
1,1-dichloroethane	<8	<160	<160	<160	<160	<160	<160	<160	<160	<160			
1,2-dichloroethane	<8	T(151)	<151	T(151)	<151	T(151)	T(151)	T(151)	T(151)	T(151)			
1,1,1-trichloroethane	<5	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)	T(217)			
1,1,2-trichloroethane	<5	<167	<167	<167	<167	<167	<167	<167	<167	<167			
trichloroethylene	<5	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)	T(155)			
tetrachloroethylene	<7	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)	T(19)			
1,1,1,2-tetrachloroethane	<6	<16	<16	<16	<16	<16	<16	<16	<16	<16			
1,1,2,2-tetrachloroethane	<6	<16	<16	<16	<16	<16	<16	<16	<16	<16			
pentachloroethane	<5	<6	<6	<6	<6	<6	<6	<6	<6	<6			
hexachloroethane	<5	<6	<6	<6	<6	<6	<6	<6	<6	<6			
chlorobenzene	<15	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)	T(18)			
o-dichlorobenzene	<10	T(9)	<9	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)			
m-dichlorobenzene	<10	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)	T(9)			
p-dichlorobenzene	<9	<7	<7	<7	<7	<7	<7	<7	<7	<7			
1,2,4-trichlorobenzene	<6	<7	<7	T(7)	<7	<7	<7	<7	<7	<7			
1,3,5-trichlorobenzene	<5	<6	<6	<6	<6	<6	<6	<6	<6	<6			
1,2,3-trichlorobenzene	<6	<7	<7	<7	<7	<7	<7	<7	<7	<7			
vinylidene chloride	<10	<213	<213	<213	<213	<213	<213	<213	<213	<213			

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is listed preceded by <.

B = blank control. Values are in ng/cartridge.

Table 22. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM
FRONT ROYAL, VA ---- TRIP 1

Chemical	B	Period/Location									
		P1/L1	P1/L2	P1/L3	P1/L4	P2/L3	P2/L5	P3/L2	P3/L3	P3/L6	
benzene	<3	722	231	161	52	2481	1167	426	3526	142	
toluene	<3	171	265	151	96	3290	1066	302	4659	280	
naphthalene	<3	18	26	13	<13	196	210	26	196	71	
acetophenone	<10	<14	256	94	123	654	329	127	655	283	
n-octanal	<10	49	47	T(22)	<44	69	T(22)	31	77	37	
benzophenone	<10	32	40	T(15)	<44	17	83	55	<17	52	
phenol	<15	45	80	15	30	137	114	44	137	77	
diphenyl ether	<10	14	30	T(15)	<44	16	<44	<22	T(17)	T(31)	
ethyl acetate	<7	T(97)	T(21)	T(146)	<65	194	<97	T(97)	292	<65	
cyanobenzene	<5	<10	<15	<8	<22	<9	<22	<11	<9	<15	
dimethyldisulfide	<8	<163	<235	<238	<113	<14	<35	<163	<235	<25	

Values in ng/m³.

T = trace, values in parentheses are detection limits

Where no compound was detected, the detection limit is listed preceeded by <.

B = blank control. Values are in ng/cartridge.

Table 23. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM FRONT ROYAL, VA^a
 ---TRIP 2

Chemical	B	Period/Location									
		P1/L1	P1/L2	P1/L3	P1/L4	P1/L5	P2/L1	P2/L2	P2/L3	P2/L5	
benzene	<3	6334	574	9500	24389	55	685	611	10111	2667	
toluene	<3	3957	400	8547	3918	45	461	387	10384	2767	
naphthalene	<3	416	27	367	634	T(7)	34	24	442	154	
acetophenone	<10	209	70	240	3721	T(22)	27	48	761	327	
n-octanal	<10	30	24	132	524	T(22)	50	T(22)	157	107	
benzophenone	<10	<25	24	<63	<164	T(22)	T(26)	T(15)	50	179	
phenol	<15	128	34	462	967	T(33)	T(39)	12	225	77	
diphenyl ether	<10	T(25)	24	<63	<164	T(22)	<26	<15	<14	35	
ethyl acetate	<7	118	T(97)	667	583	<97	T(97)	T(97)	361	500	
cyanobenzene	<5	<36	12	10	<82	<11	<13	<10	<30	<30	
dimethyldisulfide	<8	T(489)	<163	<490	<490	<163	T(163)	<163	<489	<489	

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is preceded by <.

B = blank control. Values are in ng/cartridge.

Table 24. ESTIMATED LEVELS OF VOLATILE ORGANICS IN AMBIENT AIR FROM FRONT ROYAL, VA^a---
TRIP 3

Chemical	B	Period/Location									
		P1/L2	P1/L4	P1/L7	P1/L8	P1/L9	P2/L2	P2/L7	P2/L8	P2/L9	
benzene	<3	380	583	778	509	592	231	518	361	481	
toluene	<3	140	395	322	269	113	160	61	421	569	
naphthalene	<3	11	42	24	45	8	11	30	33	21	
acetophenone	<10	9	76	126	91	146	69	90	71	40	
n-octanal	<10	T(18)	T(21)	T(17)	T(18)	T(18)	T(18)	40	<18	18	
benzophenone	<10	T(12)	<21	<10	<16	19	18	<9	<18	<8	
phenol	<15	12	13	20	T(23)	26	11	7	17	T(12)	
diphenyl ether	<10	<14	<21	<10	<11	<14	19	<9	<18	<8	
ethyl acetate	<7	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	T(43)	
cyanobenzene	<5	22	T(10)	34	13	28	T(9)	22	<9	<8	
dimethyldisulfide	<8	<77	<77	<77	<77	<77	<77	<77	<77	T(77)	

Values in ng/m³.

T = trace, values in parentheses are detection limits.

Where no compound was detected, the detection limit is preceded by <.

B = blank control. Values are in ng/cartridge.

night-time effects discussed above may have been applicable to this sample. The volatile organic levels during Trip 3 were generally low.

The most striking feature of the halogenated organic quantitation is the high levels of the C₁ halocarbons (methylene chloride, chloroform and carbon tetrachloride). Levels of 1,2-dichlorethylene were significant in two samples (Trip 2, P2/L3 and P2/L5) which were collected overnight. Levels of vinylidene chloride were significant in two samples collected during Trip 1 (P2/L3 and P3/L2).

Semivolatiles

The compounds identified in the toluene and methanol extracts of the <1.7 μ fraction of air particulate from Front Royal are presented in Appendix F. The corresponding peaks are shown in the total ion current (TIC) chromatograms in Appendix F. The computer scales the TIC chromatograms to the most intense peak, so quantitative comparison of the two fractions is not possible.

DISCUSSION

Many more compounds were identified with greater frequency in the Kanawha Valley than in the Shenandoah Valley. This is especially noticeable in the pollutants potentially arising from industrial activity (halogenated and oxygenated compounds). Many compounds, including the aromatics, result from combustion (e.g. automobile exhaust) or other sources which could be considered ubiquitous. This qualitative comparison is in keeping with the greater industrial diversity and higher population density of the Kanawha Valley.

In contrast to the qualitative data, the quantitative data showed much higher levels of most organic pollutants in the Shenandoah Valley than in the Kanawha Valley. This is especially noteworthy, since the Shenandoah Valley is broader and less well-defined and is therefore not expected to be as good an emission reservoir as the Kanawha Valley. The high levels in the Shenandoah Valley were found on both Trips 1 and 2, implying that the levels found are not fortuitous.

The origins of the high levels of pollutants in the Shenandoah and Kanawha Valleys are not discernible from these data, since wind directions were inconsistent during most of the sampling.

It appears from the results presented here that the highest concentrations of pollutants in the Shenandoah Valley occur at night. Therefore, future sampling efforts should make more direct comparisons between day and night levels at the same locations.

SECTION 8

QUALITY CONTROL

Quality control was recognized as an integral and primary component of this program. As such, a rigorous quality assurance program was established to prevent contamination or loss of sample, mislabeling, and to provide estimates on the accuracy of the data. The essential features of the quality control program are discussed below.

SAMPLING

The quality control program used for the sampling of ambient air included sample and data logging, reagent and glassware control, and control samples as discussed below.

Sample Collection

During sample collection, a sample data sheet (Figure 11) was maintained for each sample. The sampling locations for each sampling period were recorded on a detailed area map. The coded form contained information such as date and time of sampling, locations, sampling parameters and meteorological information. The alpha-numeric sample code was also fixed directly to the sample container at that time.

Following each day's sample collection, the protocol sheets and sample labels were independently reviewed by two field personnel to assure that all information was logged in, that the codes were self-consistent and that there was no duplication. Upon returning to the laboratory, the samples were again checked for proper labeling. Upon submission for analysis, the samples were logged in by the GC/MS/COMP operator and a running account of sample analysis and data output maintained. When the sample analysis and data output were completed, the data were returned to the Project Director and logged in.

Each sample was collected on duplicate cartridges in parallel. Thus, additional quality assurance was provided not only in case of sample damage, but also for confirmatory analysis if necessary.

FIELD SAMPLING PROTOCOL

Date: _____

() () () () ()
 Project No. Operator Seq. Sampler/Rationale State

Municipality _____ ()

Location _____

Site _____ ()

Sample Code _____

No.	Dimensions (cm)	Sorbent	Date/Analytical Procedure
_____	_____	(M)	_____
_____	_____	(M)	_____
_____	_____	(M)	_____
_____	_____	(M)	_____

DC Amps _____ Sampling Rate (LPM) _____ Vacuum ("Hg) _____

Rationale: Qual. Anal (F) _____ End: Time _____ ft³

Quant. Anal. (E) _____ Calibration (C) _____ Start: Time _____ ft³

Experimental: Lab (L) _____ Field (X) _____ Total: (min). _____ ft³

Remarks _____ Volume Air/Cartridge: _____

_____ 0.0283 (ft³) = _____ (M³)

_____ No. Split _____

MAP:

Time _____ Temp. Wet. _____ Dry _____

Rel. Humid _____ % Wind Dir./Speed _____ /

Cloud _____ Odor _____

Remarks _____

Time _____ Temp. Wet. _____ Dry _____

Rel. Humid _____ % Wind Dir./Speed _____ /

Cloud _____ Odor _____

Remarks _____

Time _____ Temp. Wet. _____ Dry _____

Rel. Humid _____ % Wind Dir./Speed _____ /

Cloud _____ Odor _____

Remarks _____

Time _____ Temp. Wet. _____ Dry _____

Rel. Humid _____ % Wind Dir./Speed _____ /

Cloud _____ Odor _____

Remarks _____

Figure 11. Field Sampling Protocol Data Sheet.

Reagent and Glassware Control

Reagent and glassware control was required in order to minimize contamination. Sample containers, glassware, etc. were cleaned with Isoclean[®], rinsed with deionized-distilled water and heat treated at 450-500°C to insure the removal of all traces of organic compounds. Solvents were redistilled in glass in our laboratories prior to their use.

Quality Control Samples

Blank sampling cartridges and control cartridges loaded with known amounts of standards were prepared for each sampling trip. Half of the samples were designated "lab blanks/controls" and remained in the laboratory, the other half were designated "field blanks/controls", and were carried to the field in the same containers as the sampling cartridges. The quality control scheme is outlined in Table 25. This procedure not only provided a check of possible contamination during transportation and storage, but also allowed calculation of overall recoveries during the storage and analysis phases.

SAMPLE WORKUP AND ANALYSIS

Volatiles Collected on Tenax GC Cartridges

The quality assurance program consisted of analysis of controls and blanks, cross-checking data interpretation, and validation of methodology.

The results of the blank analyses are included with the quantitation results (Tables 15, 16, 19, 21-24). The recoveries of selected organic compounds from Tenax GC cartridges are listed in Table 10. The results from Trip 3 are not included because the standards were improperly loaded onto the cartridges. The recoveries shown are very good, considering that each cartridge was stored at ambient temperature for up to one week during sampling. These results indicate that sample loss from the cartridges during storage is minimal.

The qualitative data presented in Appendices C-F were independently checked after interpretation.

The entire method has been previously validated. (1-7,11,12)

Highly Volatile Compounds Collected on Carbon Cartridges

The quality control program for these samples was essentially the same as for the samples collected on Tenax GC. The recoveries of compounds on

Table 25 . CONTROL SAMPLES FOR EACH FIELD SAMPLING TRIP.

Sample Type	Blank ^a (Lab)	Blank ^b (Field)	Controls ^a (Lab)	Controls ^b (Field)	Total
Tenax Cartridges	2	2	2 ^c	2 ^c	8
Carbon Cartridges	2	2	2 ^d	2 ^d	8

^aRemain in laboratory, stored with samples on return.

^bTravel with samples to the field and return.

^cCartridges were loaded with benzene (240.5 ng), methylene chloride (300 ng), toluene (110 ng), 1,1,1-trichloroethane (35 ng), chloroform (200 ng) and methyl ethyl ketone (194 ng).

^dCartridges were loaded with methyl chloride (310 ng) and methyl bromide (100 ng).

the controls were not quantitated since no compounds of interest were found in the field samples. The method has been thoroughly validated on previous contracts. (7,11,12)

Particulate Collected on MAS

Since there was no suitable method of preparation of control and blank samples and quantitation was not attempted, no quality control samples were used.

As discussed above, the extraction method was validated for a broad range of organic compounds.

The data interpretation is described above. It was necessary to employ two independent interpreters to assure that identifications were correct. This procedure was especially critical for the semi-volatiles (vis á vis the compounds collected on Tenax GC) due to the large number of possible compounds present, and the relative state of the art.

Summary

In summary, measures were taken to assure that both the qualitative and quantitative data generated under this study are accurate and complete.

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APPENDIX A

SAMPLING AND ANALYSIS FOR VOLATILE ORGANICS IN AMBIENT AIR

APPENDIX A
SAMPLING AND ANALYSIS FOR VOLATILE ORGANICS IN AMBIENT AIR

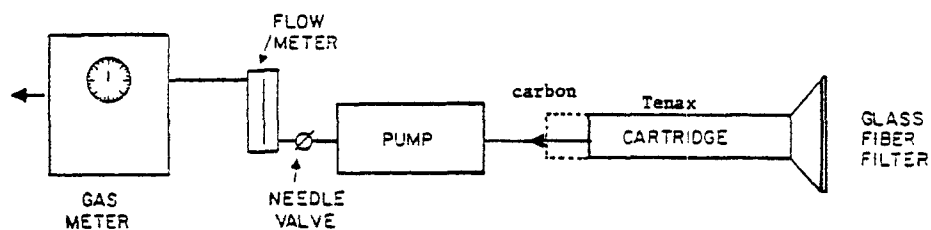
1.0 Principle of Method

Volatile organic compounds are concentrated from ambient air on Tenax GC in a short glass tube (1-3). Recovery of the volatile organics is accomplished by thermal desorption and purging with helium into a liquid nitrogen cooled nickel capillary trap (1,2,4) and the vapors then introduced onto a high resolution glass gas chromatographic column where the constituents are separated from each other (2,5). Characterization and quantitation of the constituents in the sample are accomplished by mass spectrometry, either by measuring the intensity of the total ion current signal or mass fragmentation (2,6). The collection and analysis systems are shown in Figure A-1.

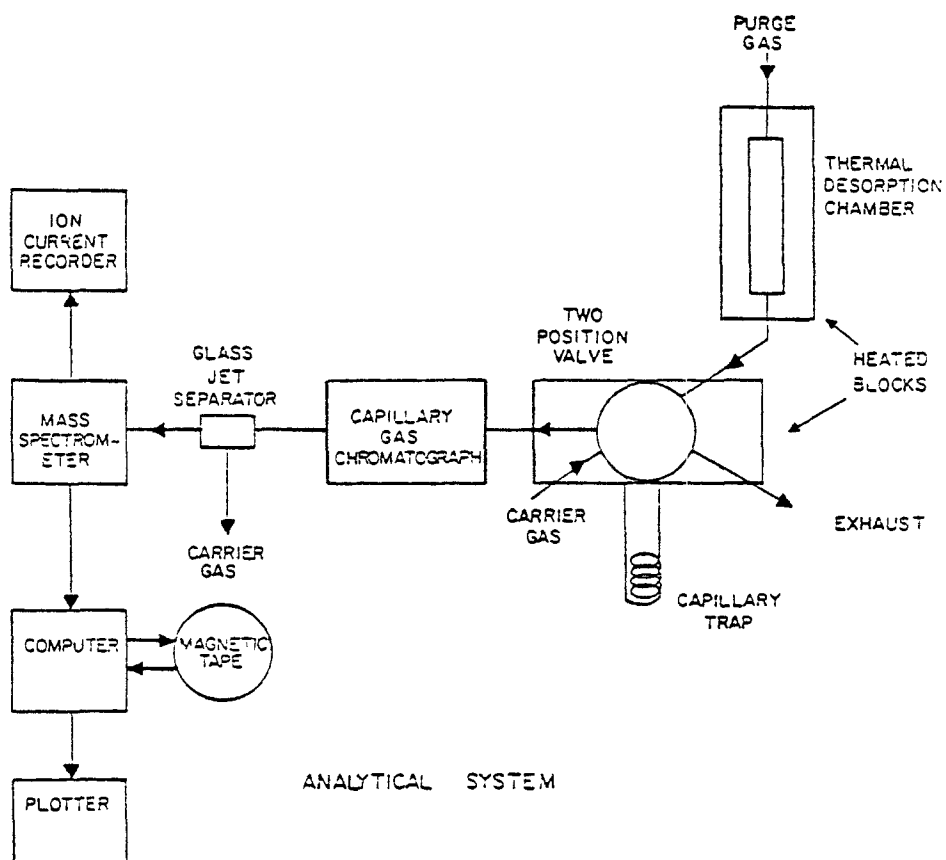
2.0 Range and Sensitivity

The linear range for the analysis of volatile organic compounds depends upon two principal features. The first is a function of the breakthrough volume of each specific compound trapped on the Tenax GC sampling cartridge, and the second is related to the inherent sensitivity of the mass spectrometer for each organic compound (2,7). Thus, the range and sensitivity is a direct function of each compound which is present in the original ambient air. The linear range for quantitation on the gas chromatograph/mass spectrometer/computer (GC/MS/COMP) is generally three orders of magnitude. Table A-1 lists the overall theoretical sensitivity for some examples of volatile organics which is based on these two principles (7).

The sensitivity of this technique for the very volatile compounds (C_1 to C_5) is inadequate for the purpose of this study. Alternate methods for their collection and analysis are suggested.



VAPOR COLLECTION SYSTEM



ANALYTICAL SYSTEM

Figure A-1. Vapor collection and analytical systems for analysis of organic vapors in ambient air.

Table A-1. OVERALL THEORETICAL SENSITIVITY OF HIGH RESOLUTION
GAS CHROMATOGRAPHY/MASS SPECTROMETRY/COMPUTER ANALYSIS
FOR ATMOSPHERIC POLLUTANTS

Chemical Class	Estimated Detection Limit ^a	ng/m ³		ppt
Halogenated hydrocarbon	Vinyl bromide	250		57
	Bromoform	0.340		0.03
	Bromodichloromethane	1.300		0.22
	Dibromochloromethane	0.667		0.07
	1-Bromo-2-chloroethane	1.00		0.67
	Allyl bromide	5.00		1.04
	1-Bromopropane	5.200		1.06
	1-Chloro-3-bromopropane	0.150		0.01
	1-Chloro-2,3-dibromopropane	~0.100		<0.01
	1,1-Dibromo-2-chloropropane	~0.100		<0.01
	1,2-Dibromoethane	0.530		0.07
	1,3-Dibromopropane	~0.100		~0.01
	Epichlorohydrin	9.600		2.50
	(1-Chloro-2,3-epoxypropane)			
	Epibromohydrin	0.300		0.05
	(1-Bromo-2,3-epoxypropane)			
	Bromobenzene	0.100		0.02
	Methyl bromide	500		135
	Methyl chloride	2000		1000
	Vinyl chloride	800		333
	Methylene chloride	700		200
	Chloroform	200		420
	Carbon tetrachloride	250		400

(continued)

Table A-1 (continued)

Chemical Class	Compound	Estimated Detection Limit ^a	
		ng/m ³	ppt
Halogenated hydrocarbon (cont'd)	1,2-Dichloroethane	32	8.15
	1,1,1-Trichloroethane	66	12.45
	Tetrachloroethylene	2.5	0.38
	Trichloroethylene	10	1.92
	1-Chloro-2-methylpropene	62	21.5
	3-Chloro-2-methylpropene	62	21.5
	3-Chloro-1-butene	83	28.8
	Allyl chloride	83	28.8
	4-Chloro-1-butene	38	13.2
	1-Chloro-2-butene	13	4.5
Halogenated ethers	Chlorobenzene	2.10	0.47
	<u>o</u> -Dichlorobenzene	1.00	0.06
	<u>m</u> -Dichlorobenzene	0.75	0.01
	Benzylchloride	0.65	0.01
	2-Chloroethyl ethyl ether	4.15	0.97
Nitrosamines	Bis-(chloromethyl)ether	1.0	1.10
	N-Nitrosodimethylamine	5.0	1.67
	N-Nitrosodiethylamine	3.0	0.74
Oxygenated	Acrolein	~100	56.5
	Glycidaldehyde	~59	19.5
	Propylene oxide	~60	25.5
	Butadiene, 1,3-diene	~70	6.7

Table A-1 (continued)

Chemical Class	Compound	Estimated Detection Limit ^a	
		ng/m ³	ppt
Oxygenated hydrocarbons (continued)	Cyclohexene oxide	~10	2.5
	Styrene oxide	2	0.415
	Acetophenone	~2	~0.415
	β-Propiolactone	~3	~1.2
Nitrogenous Compounds	Nitromethane	8	~2.4
	Aniline	3.0	0.78
Sulfur Compounds	Diethyl sulfate	~50	-
	Ethyl methane sulfate	~5.0	-

^aLimits are calculated on the basis of the breakthrough volume for 2.2 g of Tenax GC, capillary column performance and sensitivity of the mass spectrometer to that compound in the mass fragmentography mode of most intense ion.

3.0 Interferences

The potential difficulties with this technique are primarily associated with those cases where isomeric forms of a particular substance cannot be resolved by the high resolution chromatographic column and the mass cracking pattern of each of the isomers is identical. An example of such a problem is seen with the C₅-alkyl aromatics of which there are 53 isomers. As the number of carbon atoms increase in the hydrocarbons and aromatics, the number of potential isomers become increasingly large and difficult to completely resolve by gas chromatography and/or by their corresponding mass cracking patterns. However, differentiation between the hydrocarbons, that is alkanes, alkenes, aromatics, oxygenated, etc. can be made. Known background compounds include phthalate esters; silanes, phosphines and thio-phosphines (from the SCOT column); 2,2,4-trimethylpenta-1,3-diol-diisobutyrate ("SNOOP"); fluorocarbon refrigerants; and acetic acid (Tenax GC decomposition product).

Interferences in quantitation can usually be avoided by properly setting the computer S/N threshold.

4.0 Reproducibility

The reproducibility of this method has been determined to range from ± 10 to ± 30 percent of the relative standard deviation for different substances when replicate sampling cartridges are examined (5). The inherent analytical errors are a function of several factors: (1) the ability to accurately determine the breakthrough volume for each of the identified organic compounds, (2) the accurate measurement of the ambient air volume sampled, (3) the percent recovery of the organic from the sampling cartridge after a period of storage, (4) the reproducibility of thermal desorption for a compound from the cartridge and its introduction into the analytical system, (5) the accuracy of determining the relative molar response ratios between the identified substance and the external standard used for calibrating the analytical system, (6) the reproducibility of transmitting the sample through the high resolution gas chromatographic column, and (7) the day-to-day reliability of the ms-comp system (1-8).

The accuracy of the analysis is generally $\pm 30\%$, however, the accuracy is dependent on the chemical and physical nature of the compound (2,8).

5.0 Advantages and Disadvantages of the Method

The gas chromatograph/mass spectrometer, interfaced with a glass jet separator is extremely sensitive and specific for the analysis of many organic compounds in ambient air. High resolution gas chromatographic separation provides adequate resolution of the substances found in ambient air for their subsequent quantification. The combination of high resolution gas chromatographic column and the selection of specific or unique ions representing the various compounds identified in air samples yields a relatively specific assay method for these compounds (1-8).

Collected samples can be stored up to one month with less than 10% losses for most of the chemical classes (2,8). Because some of the compounds of interest may be hazardous to man, it is extremely important to exercise safety precautions in the preparation and disposal of liquid and gas standards, cleaning of used glassware, etc. and the analysis of air samples.

Since the mass spectrometer cannot be conveniently mobilized, sampling must be carried out away from the instrument.

The efficiency of air sampling increases as the temperature of ambient air decreases (i.e., sensitivity increases) (8).

The retention of water by Tenax is low, its thermal stability is high and its background is negligible allowing sensitive analysis (1,2,5,8).

6.0 Apparatus

6.1 Sampling Cartridges

The sampling tubes are prepared by packing a 10 cm long x 1.5 cm i.d. glass tube with 6.0 cm of 35/60 mesh Tenax GC, placing glass wool in the ends to provide support (2,5). Virgin Tenax (or material to be recycled) is extracted in a Soxhlet extractor for a minimum of 48 hours with methanol and pentane prior to preparation of cartridge samplers (2,5). After purification of the Tenax GC sorbent and drying in a vacuum oven at 100°C for 16 hr at a vacuum of 28 inches of water, all the sorbent material is meshed to provide a 35/60 particle size range. Cartridge samplers are then prepared and conditioned at 270°C with helium flow at 30 ml/min for 30 minutes. The conditioned cartridges are transferred to Kimax[®] (2.5 cm x 150 cm) culture tubes, immediately sealed using Teflon lined caps, and cooled. This procedure is performed in order to avoid recontamination of the sorbent bed (2,5).

Cartridge samplers with longer beds of sorbent may be prepared using a proportional increase in the amount of Tenax GC in order to achieve a larger breakthrough volume for each compound and thus increasing the overall sensitivity of the technique (8).

6.2 Gas Chromatographic Column

A 0.35 mm i.d. x 100 m glass SCOT capillary column coated with SE-30 stationary phase and 0.1% benzyltriphenylphosphonium chloride is used for effecting the resolution of the volatile organic compounds (5). The capillary column is conditioned for 48 hr at 245°C at a 2.25 ml/min helium flow.

A glass jet separator on a Varian-MAT CH-7 GC/MS/COMP system is employed to interface the glass capillary column to the mass spectrometer. The glass jet separator is maintained at 240°C (2.5).

6.3 Inlet Manifold

An inlet manifold for thermally recovering vapors trapped on Tenax sampling cartridges is employed and is shown in Figure A-1 (1,2,4,5).

6.4 Gas Chromatograph

A Varian 1700 gas chromatograph is used to house the glass capillary column and is interfaced to the inlet manifold (Fig A-1).

6.5 Mass Spectrometry/Computer

A Varian-MAT CH-7 mass spectrometer with a resolution of 2,000 equipped with a single ion monitoring capability is used in tandem with the gas chromatograph (Fig. A-1). The mass spectrometer is interfaced to a Varian 620/L computer (Fig. A-1).

7.0 Reagents and Materials

All reagents used are analytical reagent grade.

8.0 Procedure

8.1 Cleaning of Glassware

All glassware, sampling tubes, cartridge holders, etc. are washed in Isoclean[®]/water, rinsed with deionized distilled water, acetone and air dried. Glassware is heated to 450-500°C for 2 hours to insure that all organic material has been removed prior to its use.

8.2 Collection of Halogenated Hydrocarbons in Ambient Air

Continuous sampling of ambient air is accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Fig. A-1, ref. 2). Flow rates are maintained at 1-10 l/min are available with the system. Flow rates are generally maintained at 1 l/min using critical orifices, and the total flow is monitored through a calibrated flow meter. The total flow is also registered by a dry gas meter. Concomitant with these parameters the temperature is continuously recorded with a Meteorology Research Incorp. Weather Station since the breakthrough volume is important in order to obtain quantitative data on the volatile organics. This portable sampling unit operates on a 12 volt storage battery and is capable of continuous operation up to a period of 24 hours. However, in most cases, the sampling period will consist of 1 to 3 hours at the rates which will be employed in the field. This portable sampling unit will be utilized for obtaining "high volume" samples. Duplicate cartridges are deployed on each sampling unit utilizing a sampling head as shown in Figure A-2.

In addition to the Nutech samplers five duPont personnel samplers are used to sample "low volumes" of ambient air as well as long term integrated samples (12-36 hr). Identical Tenax GC sampling cartridge are employed in this case, and sampling is conducted in duplicate. The flow rate is balanced between duplicate cartridges using critical orifices to maintain a rate of 25 or 100 ml/min/cartridge.

For large sample volumes it is important to realize that a large volume of air may cause elution of compounds through the sampling tube if their breakthrough volume is exceeded. The breakthrough volumes of some volatile organics are shown in Table A-2 (2,4,7,8). These breakthrough volumes have been determined by a previously described technique (2). The breakthrough volume is defined as that point at which 50% of a discrete sample introduced into the cartridge is lost. Although the identity of a compound during ambient air sampling is not known (therefore also its breakthrough volume) the compound can still be quantified, after identification by GC/MS/COMP, once the breakthrough volume has been established. Thus the last portion of the sampling period corresponding to the breakthrough volume is selected for calculating their concentration.

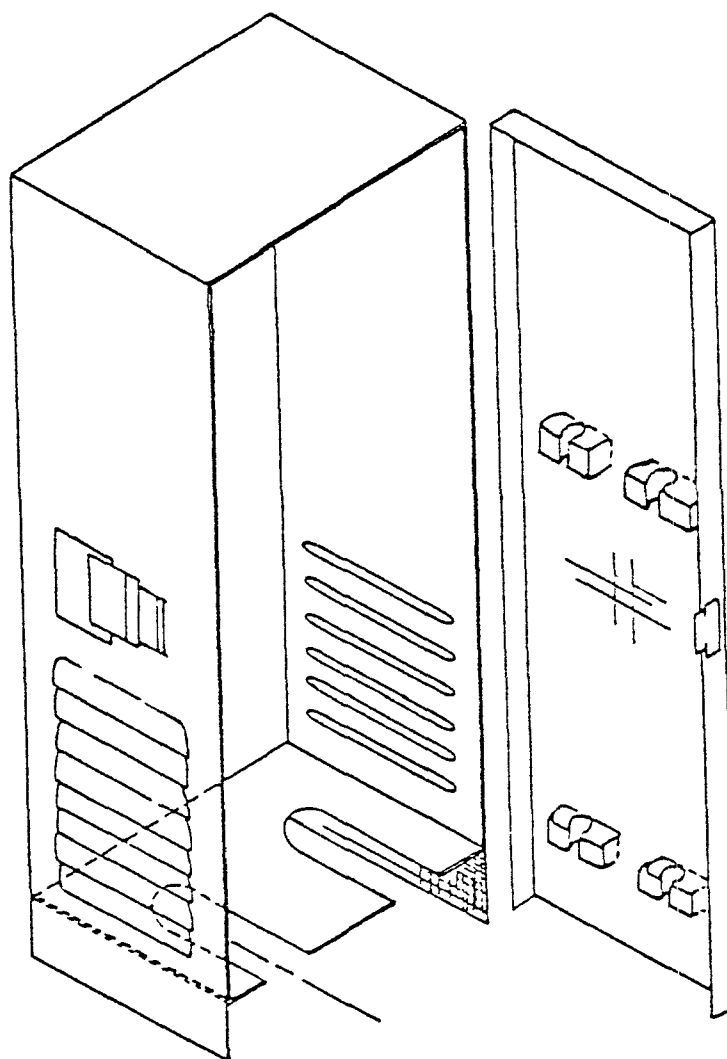


Figure A-2. Sampling head for housing cartridge sampling train.

Table A-2. BREAKTHROUGH VOLUMES FOR SEVERAL ATMOSPHERIC POLLUTANTS¹

Chemical Class	Compound	b.p. (°C)	Temperature (°F)							
			50	60	70	80	90	100		
halogenated hydrocarbon	methyl chloride	-24	0.8	0.6	0.5	0.4	0.3	0.25		
	methyl bromide	3.5	3	2	2	1	1	0.9		
	vinyl chloride	13	2	1.5	1.25	1.0	0.8	0.6		
	methylene chloride	41	11	9	7	5	4	3		
	chloroform	61	42	31	24	18	13	10		
	carbon tetrachloride	77	34	27	21	16	13	10		
	1,2-dichloroethane	83	53	41	31	23	18	14		
	1,1,1-trichloroethane	75	23	18	15	12	9	7		
	tetrachloroethylene	121	361	267	196	144	106	78		
	trichloroethylene	87	90	67	50	38	28	21		
	1-chloro-2-methylpropene	68	26	20	16	12	9	7		
	3-chloro-2-methylpropene	72	29	22	17	13	10	8		
	1,2-dichloropropane	95	229	162	115	81	58	41		
	1,3-dichloropropane	121	348	253	184	134	97	70		
	epichlorohydrin (1-chloro-2,3-epoxypropane)	116	200	144	104	74	54	39		
	3-chloro-1-butene	64	19	15	12	9	7	6		
	allyl chloride	45	21	16	12	9	6	5		
	4-chloro-1-butene	75	47	36	27	20	15	12		
	1-chloro-2-butene	84	146	106	77	56	40	29		
	chlorobenzene	132	899	653	473	344	249	181		
	o-dichlorobenzene	181	1,531	1,153	867	656	494	372		
	m-dichlorobenzene	173	2,393	1,758	1,291	948	697	510		
	benzyl chloride	179	2,792	2,061	1,520	1,125	830	612		
	bromoform	149	507	386	294	224	171	130		
	ethylene dibromide	131	348	255	188	138	101	74		
	bromobenzene	155	4,144	1,521	1,079	764	542	384		

Table A-2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F)						
			50	60	70	80	90	100	
halogenated ethers	2-chloroethyl ethyl ether	108	468	336	241	234	124	89	
	Bis-(chloromethyl)ether	-	995	674	456	309	209	142	
nitrosamines	N-nitrosodimethylamine	151	385	280	204	163	148	107	
	N-nitrosodiethylamine	177	2,529	1,836	1,330	966	700	508	
Oxygenated hydrocarbons	acrolein	53	19	14	10	8	6	4	
	glycidaldehyde	-	364	247	168	114	77	52	
	propylene oxide	34	35	24	17	11	8	5	
	butadiene diepoxide	-	1,426	1,009	714	506	358	253	
	cyclohexene oxide	132	2,339	1,644	1,153	811	570	400	
nitrogenous hydrocarbons	styrene oxide	194	5,370	3,926	2,870	2,094	1,531	1,119	
	phenol	183	2,071	1,490	1,072	769	554	398	
	acetophenone	202	3,191	2,382	1,778	1,327	991	740	
	β-propiolactone	57	721	514	366	261	186	132	
	nitromethane	101	45	34	25	19	14	11	
sulfur compounds	aniline	184	3,864	2,831	2,075	1,520	1,114	817	
	diethyl sulfate	208	40	29	21	15	11	8	
	ethyl methane sulfate	86	5,093	3,681	2,564	1,914	1,384	998	
amines	dimethylamine	7.4	9	6	4	3	2	1	
	isobutylamine	69	71	47	34	23	16	11	
	t-butylamine	89	6	5	4	3	2	1	
	di-(n-butyl)amine	159	9,506	7,096	4,775	3,105	2,168	1,462	
	pyridine	115	378	267	189	134	95	67	
	aniline	184	8,128	5,559	3,793	2,588	1,766	1,205	

Table A-2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F)						
			50	60	70	80	90	100	
esters	ethyl acetate	77	162	108	72	48	32	22	
	methyl acrylate	80	164	111	75	50	34	23	
	methyl methacrylate	100	736	484	318	209	137	90	
ketones	acetone	56	25	17	12	8	6	4	
	methyl ethyl ketone	80-2	82	57	39	27	19	13	
	methyl vinyl ketone	81	84	58	40	28	19	14	
	acetophenone	202	5,346	3,855	2,767	2,000	1,439	1,037	
aldehydes	acetaldehyde	20	3	2	2	1	0.9	0.7	
	benzaldehyde	179	7,586	5,152	3,507	2,382	1,622	1,101	
alcohols	methanol	64.7	1	1	0.8	0.6	0.4	0.3	
	n-propanol	97.4	27	20	14	10	7	5	
	allyl alcohol	97	32	23	16	11	8	6	
aromatics	benzene	80.1	108	77	54	38	27	19	
	toluene	110.6	494	348	245	173	122	86	
	ethylbenzene	136.2	1,393	984	693	487	344	243	
	cumene	152.4	3,076	2,163	1,525	1,067	750	527	
hydrocarbons	n-hexane	68.7	32	23	17	12	9	6	
	n-heptane	98.4	143	104	75	55	39	29	
	1-hexene	63.5	28	20	15	11	8	6	
	1-heptene	93.6	286	196	135	93	64	44	
	2,2-dimethylbutane	49.7	0.5	0.4	0.3	0.2	0.2	0.1	
	2,4-dimethylpentane	80.5	435	252	146	84	49	28	
	4-methyl-1-pentene	53.8	14	10	8	6	4	3	
	cyclohexane	80.7	49	36	26	19	14	10	

(continued)

Table A-2 (cont'd)

Chemical Class	Compound	b.p. (°C)	Temperature (°F)						
			50	60	70	80	90	100	
inorganic gases	nitric oxide	-	0	0	0	0	0	0	0
	nitrogen dioxide	-	0	0	0	0	0	0	0
	chlorine	-	0	0	0	0	0	0	0
	sulfur dioxide	-	0.06	0.05	0.03	0.02	0.02	0.01	0.01
	water	100	0.06	0.05	0.04	0.03	0.01	0	0

¹ Breakthrough volume is given in $\ell/2.2$ g Tenax GC used in sampling cartridges.

Previous experiments have shown that organic vapors collected on Tenax GC sorbent are stable and can be quantitatively recovered from the cartridge samplers up to four weeks after sampling when they are tightly closed in cartridge holders and placed in a second container that can be sealed, protected from light, and stored at 0°C (1,2).

8.3 Analysis of Sample

The instrumental conditions for the analysis of volatile organics on the sorbent Tenax GC sampling cartridge are shown in Table A-3. The thermal desorption chamber and the six-port valco valve are maintained at 270° and 240°C, respectively. The glass jet separator is maintained at 240°. The mass spectrometer is set to scan the mass range from 25-350. The helium purged gas through the desorption chamber is adjusted to 15-20 ml/min. The nickel capillary trap at the inlet manifold is cooled with liquid nitrogen. In a typical thermal desorption cycle a sampling cartridge is placed in the preheated desorption chamber and helium gas is channeled through the cartridge to purge the vapors into the liquid nitrogen cooled nickel capillary trap [the inertness activity of the trap has been shown in previous studies (5)]. After the desorption has been completed, the six-port valve is rotated and the temperature on the capillary loop is rapidly raised (greater than 10°/min); the carrier gas then introduces the vapors onto the high resolution glc column. The glass capillary column is temperature programmed from ambient to 240°C at 4°C/min and held at the upper limit for a minimum of 10 min. After all of the components have been eluted from the capillary column, the analytical column is then cooled to ambient temperature and the next sample is processed (2).

An example of the analysis of volatile organics in ambient air is shown in Figure A-3 and the background from a blank cartridge in Figure A-4. The high resolution glass capillary column was coated with SE-30 stationary which is capable of resolving a multitude of compounds for subsequent identification by ms-comp techniques; in this case over 120 compounds were identified in this chromatogram.

8.3.1 Operation of the MS-COMP System (Fig. A-5)

Typically, the mass spectrometer is initially set to operate in the repetitive scanning mode. In this mode the magnet is automatically scanned

Table A-3. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC 100 m glass SCOT-OV101	
50 m glass SCOT-Carbowax 20M	20-240°C, 4/C° min
	80-240°C
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	m/e 20 → 300
scan rate, automatic-cyclic	1 sec/decade
filament current	300 μ A
multiplier	6.0
ion source vacuum	$\sim 4 \times 10^{-6}$ torr

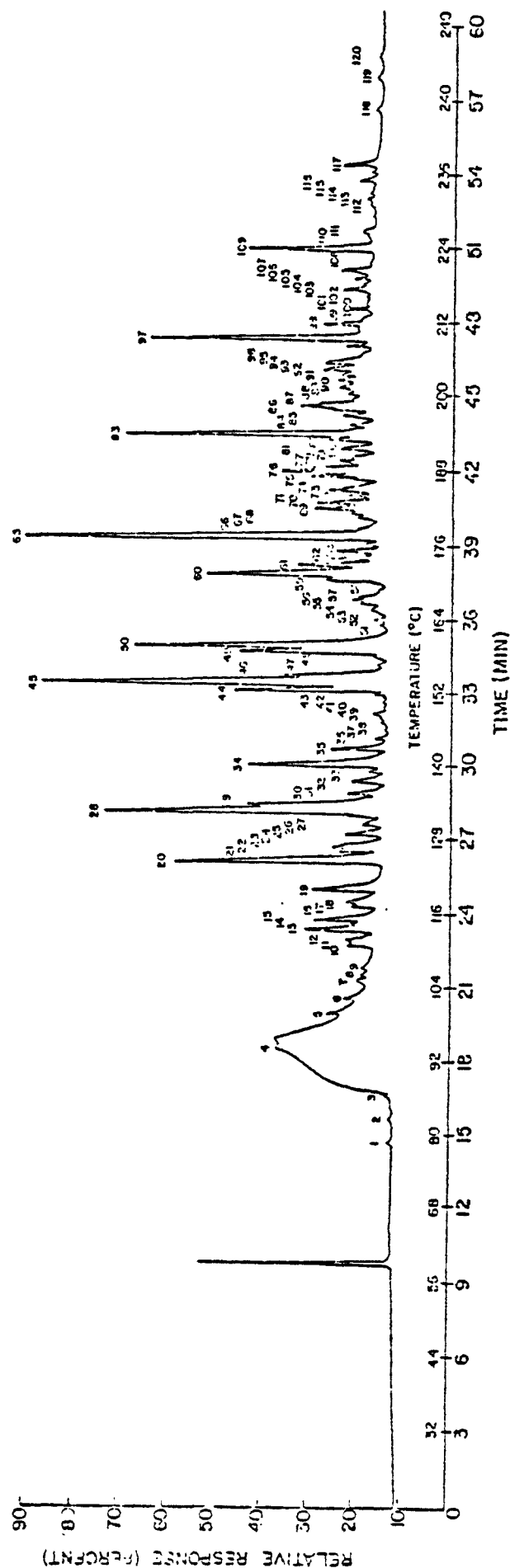


Figure A-3. Profile of ambient air pollutants for Wood River, IL using high resolution gas chromatography/mass spectrometry/computer.

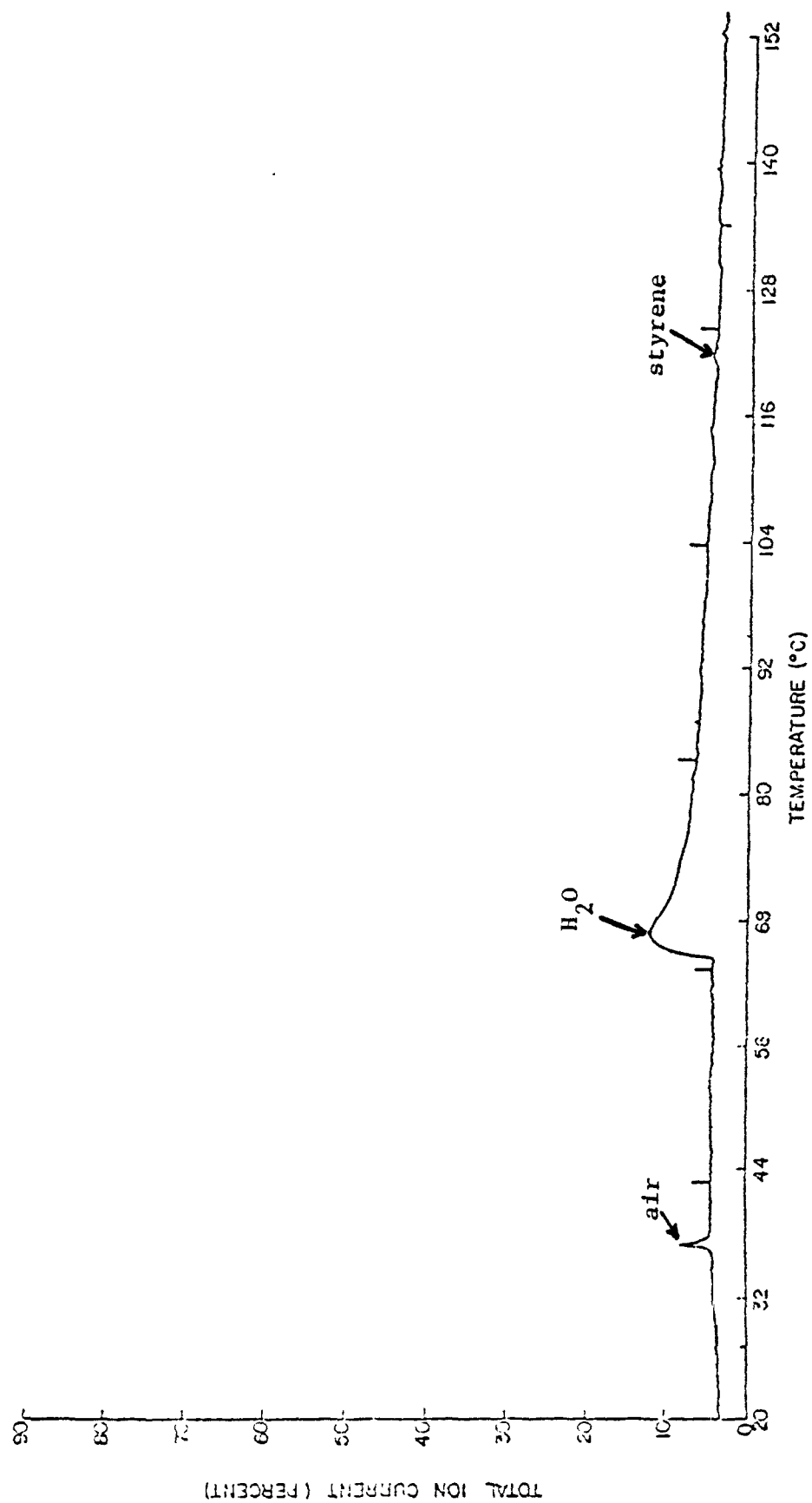


Figure A-4. Background profile for Tenax GC cartridge blank.

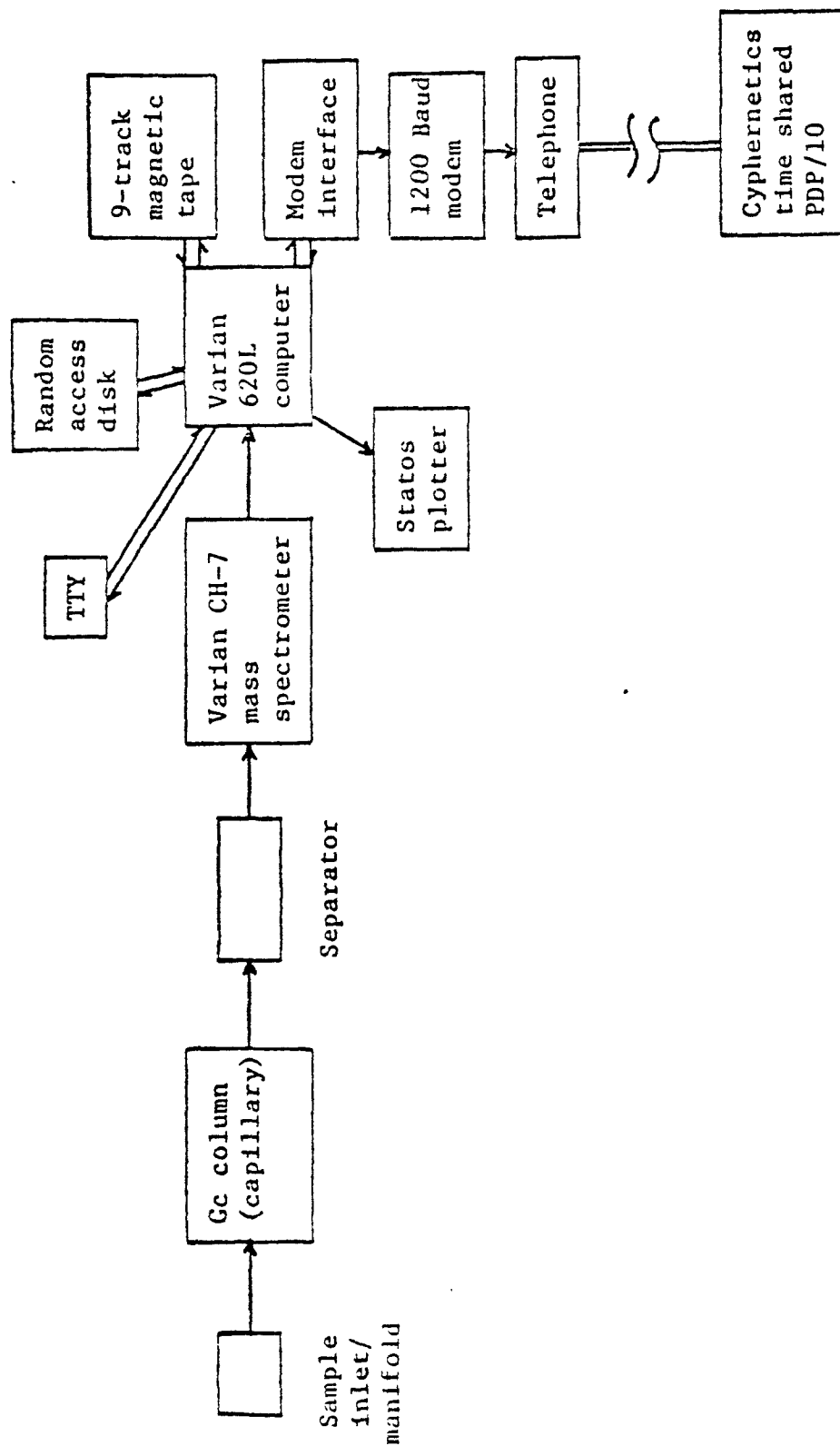


Figure A-5. Schematic diagram of gc-ms computer system

exponentially upward from a preset low mass to a high mass value. Although the scan range may be varied depending on the particular sample, the range is typically set from m/e 25 to m/e 300. The scan is completed in approximately 1.8 seconds. At this time the instrument automatically resets itself to the low mass position in preparation for the next scan, and the information is accumulated by an on-line 620/L computer and written onto magnetic tapes or the dual disk system. The reset period requires approximately 20 seconds. Thus, a continuous scan cycle of 3.8 seconds/scan is maintained and repetitively executed throughout the chromatographic run. The results is the accumulation of a continuous series of mass spectra throughout the chromatographic run in sequential fashion.

Prior to running unknown samples the system is calibrated by introducing a standard substance, perfluorokerosene, into the instrument and determining the time of appearance of the known standard peaks in relation to the scanning magnetic field. The calibration curve which is thus generated will be stored in the 620/L computer memory. This calibration serves only to calibrate the mass ion over the mass scanning range.

While the magnet is continuously scanning the sample is injected and automatic data acquisition is initiated. As each spectrum is acquired by the computer, peaks which exceed a preset threshold are recognized and reduced to centroid time and peak intensity. This information is stored in the computer core while the scan is in progress. In addition, approximately 30 total ion current values and an equal number of Hall probe signals are stored in the core of the computer as they are acquired. During the two-second period between scans this spectral information, along with the spectrum number, is written sequentially on disks, and the computer is reset for the acquisition of the next spectrum.

This procedure continues until the entire gc run is completed. By this time there are from 800-1,400 spectra on the disk which are then subsequently processed. Depending on the information required, the data may then either be processed immediately or additional samples may be run, stored on magnetic tape and the results examined at a later time.

The mass spectral data are processed in the following manner. First, the original spectra are scanned and the total ion current (TIC) information

is extracted. Then the TIC intensities are plotted against the spectrum number on the Statos 31 recorder. The information will generally indicate whether the run is suitable for further processing, since it will give some idea of the number of unknowns in the sample and the resolution obtained using the particular glc column conditions.

The next stage of the processing involves the mass conversion of the spectral peak times to peak masses which is done directly via the dual disk system. The mass conversion is accomplished by use of the calibration table obtained previously using perfluorokerosene. Normally one set of the calibration data is sufficient for an entire day's data processing since the characteristics of the Hall probe are such that the variation in calibration is less than 0.2 atomic mass units/day. A typical time required for this conversion process for 1,000 spectra is approximately 30 min.

After the spectra are obtained in mass converted form, processing proceeds either manually or by computer. In the manual mode the full set of spectral from the gc run are recorded on the Statos 31 plotter. The TIC information available at this time is most useful for deciding which spectra are to be analyzed. At the beginning of the runs where peaks are very sharp nearly every spectrum must be inspected individually to determine the identity of the component. Later in the chromatographic run when the peaks are broader, only selected scans need to be analyzed.

Identification of resolved components is achieved by comparing the mass cracking patterns of the unknown mass spectra to an eight major peak index of mass spectra (9). Individual difficult unknowns are searched through the use of the Cornell University STIRS and PBM systems. Unknowns are also submitted to the EPA MSSS system for identification. When feasible, the identifications are confirmed by comparing the cracking pattern and elution temperatures for two different chromatographic columns (SE-30 and Carbowax SCOT capillaries) for the unknown and authentic compounds. The relationship between the boiling point of the identified halogenated hydrocarbon and the elution temperature on a non-polar column (the order of elution of constituents is predictable in homologous series since the SE-30 SCOT capillary separates primarily on the basis of boiling point) is carefully considered in making structure assignments.

Mass spectra search programs are operational at the Triangle Universities Computation Center (TUCC). RTI maintains twice daily service to TUCC, which is one-quarter mile distance from the RTI campus. Additional information about each magnetic tape containing the mass spectra of halogenated hydrocarbons is entered directly into the TUCC job stream using a remote job entry processing. This is normally done using one of the five terminals located within the Analytical Sciences Laboratory. The control program contains instructions for processing selected spectra or entire gc runs. The computer program compares simultaneously either the entire library of 25,000 compounds or some subset of this library. The complete report showing the best fits for each of the unknowns is produced at TUCC and printed out at the high speed terminals located on the RTI campus.

8.3.2 Quantitative Analysis

In many cases the estimation of the level of pollutants by capillary gas chromatography in combination with mass spectrometry is not feasible utilizing only the total ion current monitor (see Fig. A-3 for example). Since baseline resolution between peaks is not always achieved, we employ techniques (previously developed under contract) whereby full spectra are obtained during the chromatographic separation step, and then selected ions are presented as mass fragmentograms using computer software programs which allow the possibility of deconvoluting constituents not resolved in the total ion current chromatogram (6). Examples are depicted in Figures A-6 and A-7 which represent an ambient air sample with a TIC profile as in Fig. A-3.

In our GC/MS/COMP system we request (from the Varian 620/L) dedicated computer mass fragmentograms for any combination of m/e ions when full mass spectra are obtained during chromatography; thus selectivity is obtained by selecting the unique ion for that particular organic substance, and this is represented versus time with subsequent use of that ion intensity for quantitation. Also, quantitation with external standards is easily achieved using the intensity of the total ion current monitor or the use of a unique mass cracking ion in the mass spectrum of that external standard. Thus, we use mass fragmentography for the quantitation of organics in ambient air when the total ion current is inadequate due to lack of complete resolution between components.

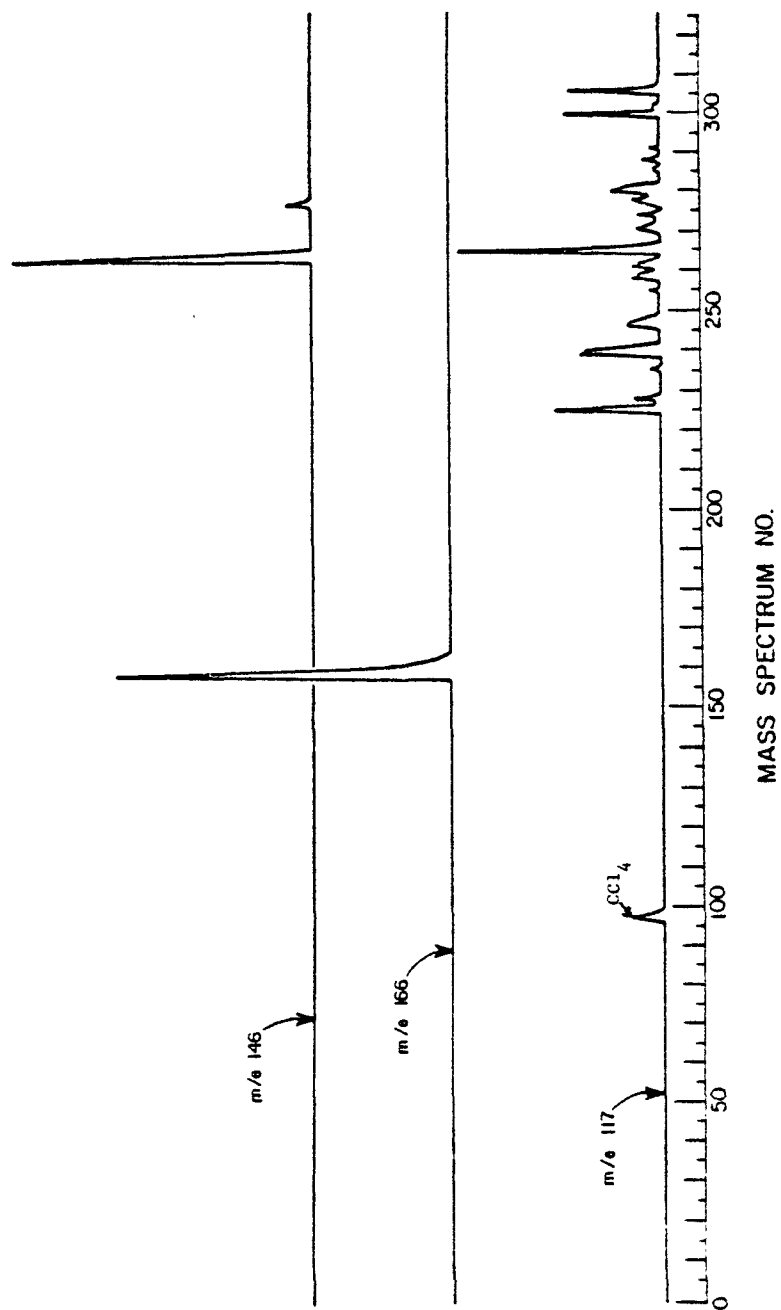


Figure A-6. Mass fragmentograms of characteristic ions representing carbon tetrachloride (m/e 117), tetrachloroethylene (m/e 166) and m-dichlorobenzene (m/e 146) in ambient air.

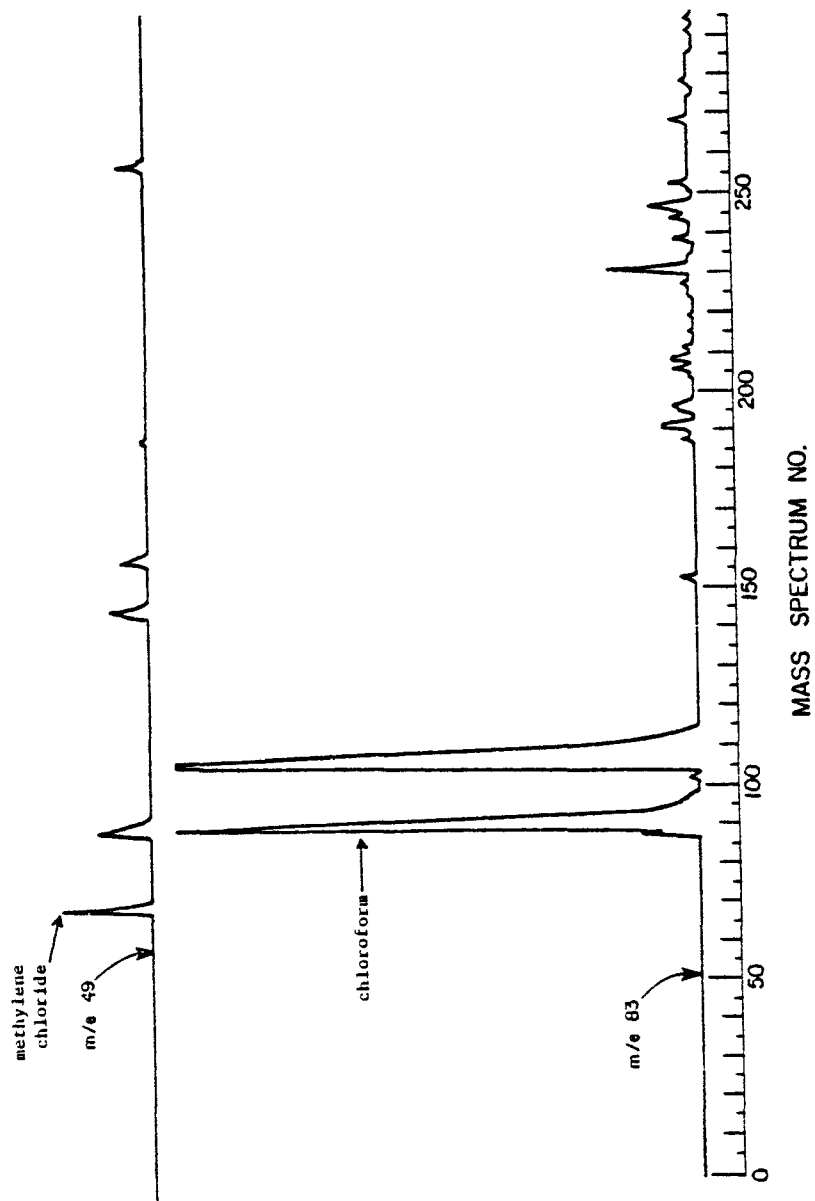


Figure A-7. Mass fragmentograms of characteristic ions representing methylene chloride (m/e 49) and chloroform (m/e 83) in ambient air.

As described previously, the quantitation of constituents in ambient air samples is accomplished either by utilizing the total ion current monitor or, when necessary, mass fragmentograms. In order to eliminate the need to obtain complete calibration curves for each compound to be quantitated, we use the method of relative molar response (RMR) factors (10). Successful use of this method requires information on the exact amount of standard added and the relationship of RMR (unknown) to the RMR (standards). The method of calculation is as follows:

$$(1) \text{ RMR}_{\text{unknown/standard}} = \frac{A_{\text{unk}}/\text{Moles}_{\text{unk}}}{A_{\text{std}}/\text{Moles}_{\text{std}}}$$

A = peak area, determined by integration or triangulation.

The value of RMR is determined from at least three independent analysis.

$$(2) \text{ RMR}_{\text{unk/std}} = \frac{A_{\text{unk}}/g_{\text{unk}}/\text{GMW}_{\text{unk}}}{A_{\text{std}}/g_{\text{std}}/\text{GMW}_{\text{std}}}$$

A = peak area, as above

g = number of grams present

GMW = gram molecular weight

Thus, in the sample analyzed:

$$(3) g_{\text{unk}} = \frac{A_{\text{unk}} \cdot \text{GMW}_{\text{unk}} \cdot g_{\text{std}}}{A_{\text{std}} \cdot \text{GMW}_{\text{std}} \cdot \text{RMR}_{\text{unk/std}}}$$

The standard can be added as an internal standard during sampling; however, since the volume of air taken to produce a given sample is accurately known, it is also possible and more practical to use an external standard whereby the standard is introduced into the cartridge just prior to its analysis. Two standards, hexafluorobenzene and perfluorotoluene are used for the purpose of calculating RMR's. From previous research, it has been determined that the retention times for these two compounds are such that they elute from the glass capillary column (SE-30) at a temperature and retention time which does not interfere with the analysis of unknown compounds in ambient air samples.

Since the volume of air taken to produce a given sample is accurately known and an external (or internal) standard is added to the sample, then the weight can be determined per cartridge (hence the concentration of the unknown). This approach for quantitating ambient air pollutants requires

that the RMR be determined for each constituent of interest. Thus, when an ambient air sample is taken, the external standard is added during the analysis at a known concentration. It is not imperative at this point to know what the RMR of each of the constituents in the sample happens to be; however, after the unknowns are identified, the RMR can be subsequently determined and the unknown concentration calculated in the original sample. In this manner it is possible to obtain qualitative and quantitative information on the same sample with a minimum of effort.

9.0 References

1. Pellizzari, E. D., Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres. Publication No. EPA-650/2-74-121, Contract No. 68-02-1228, 148 pp., July, 1974.
2. Pellizzari, E. D., Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. Publication No. EPA-600/2-76-076, Contract No. 68-02-1228, 185 pp., November, 1975.
3. Pellizzari, E. D., J. E. Bunch, B. H. Carpenter and E. Sawicki, *Environ. Sci. Tech.*, 9, 552 (1975).
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6. Pellizzari, E. D., J. E. Bunch, R. E. Berkeley and J. McRae, *Anal. Chem.*, 48, 803 (1976).
7. Pellizzari, E. D., Quarterly Report No. 1, EPA Contract No. 68-02-2262, February, 1976.
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Analytical protocol revised 5/31/78.

APPENDIX B

SAMPLING AND ANALYSIS FOR VERY VOLATILE ORGANICS (e.g., METHYL CHLORIDE
METHYL BROMIDE, VINYL CHLORIDE AND VINYL BROMIDE) IN AMBIENT AIR

APPENDIX B

SAMPLING AND ANALYSIS FOR VERY VOLATILE ORGANICS (E.G., METHYL CHLORIDE, METHYL BROMIDE, VINYL CHLORIDE AND VINYL BROMIDE) IN AMBIENT AIR

1.0 Principle of Method

Very volatile compounds (e.g., methyl chloride, methyl bromide, vinyl chloride and vinyl bromide) are concentrated from ambient air on SKC carbon in a short, glass tube (1). Recovery of these volatile halogenated hydrocarbons is accomplished by thermal desorption and purging with helium to transfer the trapped vapors from the carbon cartridge to a Tenax GC cartridge through a calcium sulfate drying tube to remove excessive amounts of water. The vapors are then transferred from Tenax into a liquid nitrogen-cooled nickel capillary trap by thermal desorption and purging with helium (2), and the vapors are introduced onto a high resolution glass, gas chromatographic column where the constituents are separated from each other (2). Identification and quantification of very volatile compounds in the sample are accomplished by mass spectrometry, either by measuring the intensity of the total ion current signal or mass fragmentography (3). The collection and analysis systems are shown in Figure B-1.

2.0 Range and Sensitivity

The linear range of the mass spectrometric signals for organic compounds depends upon two principle features. The first is a function of the breakthrough volume of each specific compound trapped on the SKC carbon sampling cartridge and the second is related to the inherent sensitivity of the mass spectrometer (3,4). Thus, the range and sensitivity is direct function of each compound. The linear range for quantification on the gas chromatograph/mass spectrometry/computer (GC/MS/COMP) is generally over three orders of magnitude. Tables B-1 and B-2 lists the breakthrough volumes for methyl chloride, methyl bromide, vinyl chloride and vinyl bromide on SKC carbon.

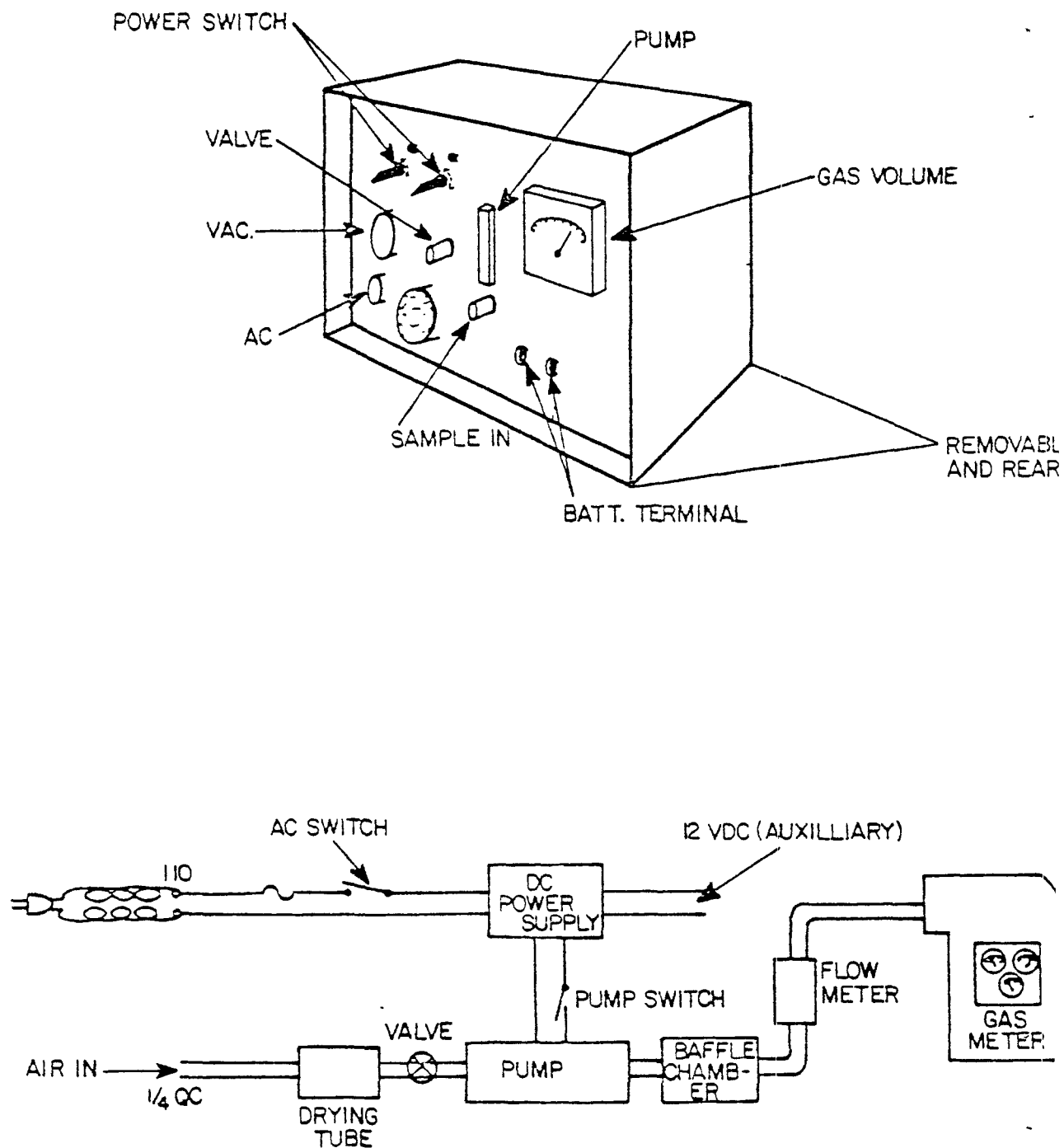


Figure B-1. Nutech Model 221-A AC-DC Sampler

Table B-1. ESTIMATION OF BREAKTHROUGH VOLUMES FOR
VINYL CHLORIDE AND VINYL BROMIDE ON SKC
CARBON (104)

Temperature °C (°F)	Vinyl Chloride		Vinyl Bromide	
	ℓ/g	ℓ/2.52 g ^a	ℓ/g	ℓ/2.52 g ^a
10 (50)	104	262	388	978
15.5 (60)	81	204	306	771
21.1 (70)	63	159	241	608
26.7 (80)	49	123	190	479
32.2 (90)	38	96	150	378
37.8 (100)	30	76	118	298

^aA 1.5 cm i.d. x 4.0 cm bed of carbon weighs 2.52 g.

Table B-2. ESTIMATION OF BREAKTHROUGH VOLUMES FOR
METHYL CHLORIDE AND METHYL BROMIDE ON
SKI CARBON (104)

Temperature °C (°F)	Methyl Chloride		Methyl Bromide	
	ℓ/g	ℓ/2.52 g	ℓ/g	ℓ/2.52 g
10 (50)	14.3	36	98	248
15.5 (60)	11.1	28	75	188
21.1 (70)	8.7	22	57	143
26.7 (80)	7.5	19	43	108
32.2 (90)	5.6	14	32	82
37.8 (100)	4.4	11	25	62

Table B-3 lists the approximate limits of detection for methyl chloride, methyl bromide, vinyl chloride and vinyl bromide based upon these breakthrough volumes. As it might be expected, the highest sensitivity is observed for vinyl bromide, and the lowest for methyl chloride. Nevertheless, the limits of detection are in the parts per trillion range.

3.0 Interferences

Because of the unique isotopic clusters for chlorine and bromine in these compounds, the background that is generally observed at their retention times on a glass capillary column will not interfere with their qualitative and quantitative analyses.

4.0 Reproducibility

The reproducibility of this method has been determined to be approximately $\pm 20\%$ of the relative standard deviation for the four compounds when replicate samples are examined (3). The reproducibility is a function of several factors. (1) The ability to accurately determine the breakthrough volume for each compound; (2) The accurate measurement of the ambient air volume sampled; (3) The percent recovery of the compound from the carbon sampling cartridge after a period of storage; (4) The reproducibility of thermally recovering each compound from the carbon cartridge and of sample introduction into the analytical system; (5) The accuracy and determination of the relative molar response ratios between the compounds of interest and the external standards used for calibrating the analytical system; (6) The relative efficiency and reproducibility of transferring the trapped vapors from the carbon sampling cartridge to the Tenax GC cartridge prior to analysis in order to remove the excessive amounts of water using calcium chloride; (7) The reproducibility of transmitting the sample through the high resolution gas chromatographic column, and (8) The day-to-day reliability of the ms/comp system (2-4).

The accuracy of analysis is generally $\pm 15\%$ of the amount determined as shown by repeated analysis of the halogenated hydrocarbons. The accuracy of the analysis is dependent upon the storage period.

Table B-3. APPROXIMATE LIMIT OF DETECTION FOR METHYL CHLORIDE, METHYL BROMIDE, VINYL CHLORIDE AND VINYL BROMIDE^a

	Ambient Air Temperature °C (°F)				
	10 (50)	15.5 (60)	21.1 (70)	26.7 (132)	32.2 (90)
Methyl chloride ^b	138 (69)	178 (89)	227 (114)	253 (132)	357 (178)
Methyl bromide ^b	8 (2.1)	11 (2.8)	14 (3.6)	18 (4.8)	24 (6.3)
Vinyl chloride ^c	48 (20)	62 (26)	79 (33)	102 (42)	131 (55)
Vinyl bromide ^c	5 (1.2)	6.5 (1.5)	8.2 (1.9)	10.5 (2.5)	28 (6.7)

^aValues are in ng/m³ (ppt)

^bEstimation of L.O.D. based on 2.52 g carbon

^cEstimation of L.O.D. based on 1.0 g carbon

5.0 Apparatus

5.1 Sampling Cartridges

The sampling tubes are prepared by packing a 10 cm long x 1.5 cm id glass tube with 2-4 cm of SKC carbon Lot No. 104, with glass wool in the ends to provide support (3,4). The carbon cartridges are conditioned at 400°C with a helium flow of approximately 30 ml/min for 30 min. The conditioned cartridges are transferred to Kimax[®] culture tubes, immediately sealed using Teflon lined caps, and cooled. This procedure is performed in order to avoid recontamination of the sorbent bed (3,4).

Cartridge samplers with longer beds of sorbents may be prepared using a proportionally increased amount of carbon in order to achieve a larger breakthrough volume for each compound, thus increasing the overall sensitivity of the technique. However, it must be noted that the percent recovery of the organic compounds significantly decreases when the amount of carbon is increased and/or when an excessive length of storage period is employed (more than a week).

5.2 Gas Chromatographic Column

A 0.35 mm i.d. x 100 m glass SCOT capillary column coated with OV-101 stationary phase and 0.1% benzyltriphenylphosphonium chloride is used for effecting resolution. The capillary column is conditioned for 48 hrs at 230°C at 1.5 - 2.0 ml/min of helium flow.

A Finnigan type glass type jet separator on a Varian MAT CH-7 GC/MS/COMP system is employed to interface the glass capillary column to the mass spectrometer. The glass jet separator is maintained at 240°C.

5.3 Inlet-Manifold

An inlet-manifold for thermally recovering compounds of interest trapped on SKC carbon sampling cartridges is employed and is shown in Figure

5.4 Gas Chromatograph

A Varian 1700 gas chromatograph is used to house the glass capillary column and is interfaced to the inlet-manifold (Figure B-1).

5.5 Mass Spectrometry/Computer

A Varian MAT CH-7 mass spectrometer with a resolution of 2000 equipped with single ion monitoring and mass fragmentography capabilities is used in tandem with the gas chromatograph (Figure B-1). The mass spectrometer is interfaced to Varian 620/L computer (Figure B-1).

6.0 Reagents and Materials

SKC carbon Lot No. 104 is from SKC Carbon Company, Boston, MA. All reagents used are analytical reagent grade and distilled in glass prior to use.

7.0 Procedure

7.1 Cleaning of Glassware

All glassware, sampling tubes, cartridge holders, etc. are washed in Isoclean[®]/water, rinsed with deionized distilled water, acetone and air dried. Glassware is heated to 450-500°C for two hours to insure that all organic material has been removed prior to its use.

7.2 Preparation of Carbon

Virgin carbon is packed into glass sampling tubes without further purification. Used carbon cartridges are not recycled.

7.3 Collection of Very Volatile Compounds in Ambient Air

Continuous sampling of ambient air is accomplished using a Nutech Model 221-A portable sampler (Nutech Corp., Durham, NC, see Figure 1). Flow rates are maintained at 1 l/min using critical orifices and the total flow is monitored through a calibrated rotameter. The total flow is also registered by a dry gas meter. Concomitant with these parameters the temperature is continuously recorded with a Meteorology Research Incorporated weather station since the breakthrough volume is important in order to obtain quantitative data on these compounds. This portable sampling unit operates on a 12-volt storage battery and it is capable of continuous operation up to a period of 24 hours. However, in most cases the sampling period consisted of one to two hours at the rates which were employed in the field. This portable sampling unit is utilized for obtaining "high volume" samples. Duplicate cartridges are deployed on each sampling unit and are in tandem with Tenax GC cartridges. The carbon cartridges serve as a backup to the Tenax GC cartridge for collecting the more highly volatile

constituents which have a low breakthrough volume on Tenax GC. A total of four portable sampling units are available for sampling ambient air surrounding the bromine industry.

In addition to the Nutech samplers, five duPont personal samplers are used to sample "low volumes" of ambient air as well as long term integrated samples (12-36 hrs). An identical SKC carbon sampling cartridge is employed in this case and sampling is conducted in duplicate. The flow rate is balanced between duplicate cartridges using critical orifices to maintain a rate of 25 or 100 ml/min per cartridge.

7.4 Analysis of Sample

The conditions for transferring very volatile organic compounds from SKC carbon sampling cartridges to Tenax GC sampling cartridges prior to instrumental analysis is shown in Table B-4. A 1.5 x 2 cm bed of calcium sulfate is used to remove the water vapor prior to retrapping of the component vapors on the Tenax GC sampling cartridge.

The instrumental conditions for the analysis of the volatile components on the sorbent carbon sampling cartridge is shown in Table B-5.

7.4.1 Operation of the MS/Comp System (Figure B-1)

The operation of the ms/comp system is identical to as that described for the Analytical Protocol under Appendix A entitled, "Sampling and Analysis for Volatile Organic Compounds in Ambient Air."

7.4.2 Quantitative Analysis

The procedure for the estimation of the level of very volatile compound by capillary gas chromatography in combination with mass spectrometry is identical to that described for the analytical protocol entitled, "Sampling and Analysis for Volatile Organics in Ambient Air".

8.0 References

1. Pellizzari, E. D. Development of Method for Carcinogenic Vapor Analysis in Ambient Atmospheres. EPA Contract No. 68-02-1228, EPA-650/2-74-121, July 1974, 148 pp.
2. Pellizzari, E. D. Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. EPA Contract No. 68-02-1228, EPA-600/2-75-076, November 1975, 187 pp.

Table B-4. PARAMETERS FOR REMOVING WATER AND TRANSFERRING
VAPORS TO TENAX GC

Parameters	Condition
Inlet-manifold	
desorption chamber	295°C
valve	200°C
CaSO ₄ drying tube (1.5 x 2.0 cm)	ambient temperature
transfer line	ambient temperature
Tenax GC cartridge (1.5 x 6.0 cm)	ambient temperature
Desorption time	10 minutes
He purge rate	10 ml/min

Table B-5. OPERATING PARAMETERS FOR GLC-MS-COMP SYSTEM

Parameter	Setting
Inlet-manifold	
desorption chamber	270°C
valve	220°C
capillary trap - minimum	-195°C
maximum	+180°C
thermal desorption time	4 min
GLC	
100 m glass SCOT-OV-101	20-240°C, 4/C° min
carrier (He) flow	~3 ml/min
transfer line to ms	240°C
MS	
scan range	$\frac{m}{e}$ 20 → 300
scan rate, automatic-cyclic	1 sec/decade
filament current	300 μ A
multiplier	6.0
ion source vacuum	$\sim 4 \times 10^{-6}$ torr

3. Pellizzari, E. D. Development of Analytical Techniques for Measuring Ambient Atmospheric Carcinogenic Vapors. EPA Contract No. 68-02-1228, 1976, in preparation.
4. Pellizzari, E. D. Identification of Atmospheric Pollutants by the Combined Techniques of Gas Chromatography/Mass Spectrometry. EPA Contract No. 68-02-2262, 1976, in preparation.

Analytical protocol revised 1/31/77.

APPENDIX C

VOLATILE AND VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN
AIR IN THE KANAWHA VALLEY, WV

Table C-1. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN
AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L2).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	10	76	hexafluorobenzene (e ⁺)
2A	55	C ₅ H ₈ isomer	11	77	n-hexane
2B	55	n-butane	11A	78	chloroform
3	57	acetaldehyde	12	82	perfluorotoluene (e ⁺)
3A	60	isopentane	12A	83	methylcyclopentane
4	61	acetone	13	88	benzene
4A	62	furan (tent.)	13A	89	cyclohexane
4B	64	vinylidene chloride (tent.)	13B	94	n-pentanal
5	65	methylene chloride	14	97	n-heptane + acetic acid
6A	67	CS ₂	15	109	toluene
7	69	C ₄ H ₈ O isomer	16	148	benzaldehyde
7A	71	methyl vinyl ketone (tent.)	17	151	phenol
8	72	2-methylpentane	17A	151	C ₁₁ H ₂₄ isomer
8A	74	C ₄ H ₈ O isomer	18	165	acetophenone
9	75	3-methylpentane			

Table C-2. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN
AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L2)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	24B	116	C ₈ H ₁₆ isomer
2A	54	C ₄ H ₈ isomer	25	117	n-octane
3	55	acetaldehyde + n-bucane (tent.)	26	118	tetrachloroethylene
3A	55	C ₄ H ₈ isomer	26A	120	C ₉ H ₂₀ isomer (tent.)
3B	59	isopentane	27	121	C ₇ H ₁₄ O isomer
4	61	acetone	28	122	C ₈ H ₁₆ isomer
4A	61	C ₅ H ₁₀ isomer	29	123	C ₉ H ₂₀ isomer
4B	62	n-pentane	29A	124	C ₉ H ₂₀ isomer
4D	64	methylene chloride	30	125	ethylcyclohexane
5B	70	C ₄ H ₆ O isomer	30A	125	C ₉ H ₂₀ isomer
6	71	2-methylpentane	30B	126	C ₉ H ₁₈ isomer
6A	72	methyl isopropyl ketone	31	128	ethylbenzene
6B	73	butanal (tent.)	32	130	xylene isomer
7	74	3-methylpentane	32A	130	C ₉ H ₂₀ isomer
8	75	hexafluorobenzene (a3)	32B	131	C ₉ H ₁₈ isomer
8A	76	n-hexane	33	132	C ₉ H ₂₀ isomer
9	77	chloroform	34	133	C ₉ H ₂₀ isomer
10	81	perfluorotoluene (a3)	35	134	styrene
10A	82	methylcyclopentane	35A	134	n-heptanal (tent.)
10B	83	1,2-dichloroethane (tent.)	36	135	o-xylene
11	84	1,1,1-trichloroethane	36A	136	C ₉ H ₁₈ isomer
11A	86	C ₆ H ₈ isomer	37	137	n-nonane
12	87	benzene	37A	138	C ₉ H ₁₈ isomer
12A	88	carbon tetrachloride	38	140	C ₉ H ₁₈ isomer
12B	89	cyclohexane	39	141	isopropylbenzene + C ₁₀ H ₂₂ isomers
13	90	2-methylhexane	39A	142	C ₁₀ H ₂₂ isomer
13A	91	acetic acid	40	142	C ₉ H ₁₆ isomer
14	92	3-methylhexane	40A	143	C ₁₀ H ₂₂ isomer
14A	93	C ₇ H ₁₄ isomer	40B	144	C ₃ -alkyl cyclohexane isomer
15	94	C ₇ H ₁₄ + C ₅ H ₁₀ O isomers	41	144	C ₁₀ H ₂₂ isomer
16	95	trichloroethylene	41A	145	C ₁₀ H ₂₀ isomer
16A	96	C ₇ H ₁₄ isomer	41B	146	C ₁₀ H ₂₂ isomer
17	97	n-heptane	42	146	benzaldehyde
17A	98	C ₇ H ₁₄ isomer	42A	146	C ₁₀ H ₂₀ isomer
18	101	methylcyclohexane	43	147	n-propylbenzene
18A	102	4-methyl-2-pentanone	44	148	ethyltoluene isomer
19	103	C ₈ H ₁₈ isomer	44A	148	C ₁₀ H ₂₂ isomer
20	108	C ₈ H ₁₆ isomer (tent.)	44B	149	C ₁₀ H ₂₂ isomer + phenol
21	109	toluene	45	150	1,3,5-trimethylbenzene
22	110	C ₈ H ₁₈ isomer	45A	150	C ₁₀ H ₂₀ isomer
22A	111	C ₈ H ₁₈ isomer	46	151	C ₁₀ H ₂₂ isomer
23	112	C ₈ H ₁₈ isomer	47	152	o-ethyltoluene
23A	113	C ₈ H ₁₆ isomer	48	153	C ₁₀ H ₂₀ isomer
24	114	C ₆ H ₁₂ isomer	48A	153	C ₁₀ H ₁₈ isomer
24A	115	C ₈ H ₁₆ isomer			

(continued)

Table C-2. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
49	154	C ₁₀ H ₂₀ isomer + n-octanal (tent.)	71A	180	C ₁₂ H ₂₄ isomer
50	154	1,2,4-trimethylbenzene	71B	181	C ₁₁ H ₂₀ isomer
50A	155	C ₁₀ H ₂₀ isomer	71C	181	C ₅ -alkyl benzene isomer
51	156	n-decane	71D	181	C ₂ -alkyl phenol isomer
52	157	dichlorobenzene isomer	71E	182	C ₄ H ₇ -benzene isomer
52A	157	C ₁₀ H ₂₀ isomer	72	182	C ₄ -alkyl benzene isomer
52B	148	C ₄ -alkyl benzene isomer	73	183	C ₅ -alkyl benzene isomer
52C	148	C ₁₁ H ₂₂ isomer	74	184	1,2,3,4-tetrahydronaphthalene
53	149	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers	74A	184	C ₅ -alkyl benzene + C ₁₃ H ₂₈ isomers
54	160	1,2,3-trimethylbenzene	75	185	C ₅ -alkyl benzene isomer
55	160	C ₁₁ H ₂₄ isomer	75A	186	C ₁₀ H ₁₆ + C ₁₃ H ₂₆ isomers
56	161	C ₁₁ H ₂₂ isomer	75B	186	C ₁₂ H ₂₄ isomer
56A	162	C ₁₀ H ₁₆ isomer	76	187	naphthalene
56B	162	indan	76A	188	C ₁₂ H ₂₄ isomer
56C	162	C ₁₁ H ₂₄ isomer	76B	189	C ₅ -alkyl benzene isomer
57	163	C ₄ -alkyl cyclohexane isomer	77	189	n-dodecane
57A	163	C ₁₁ H ₂₂ isomer	78	191	C ₅ -alkyl benzene isomer
57B	164	C ₄ -alkyl benzene isomer	79	192	C ₁₃ H ₂₈ isomer
58	164	C ₄ -alkyl benzene isomer	80	193	C ₆ -alkyl benzene isomer (tent.)
59	165	acetophenone	80A	194	C ₁₃ H ₂₆ isomer
59A	165	C ₄ -alkyl benzene isomer	81	195	C ₁₃ H ₂₈ isomer
59B	166	C ₁₁ H ₂₂ isomer	81A	195	C ₅ -alkyl benzene isomer
60	166	C ₁₁ H ₂₄ isomer	81B	197	C ₁₃ H ₂₈ isomer
61	167	C ₁₁ H ₂₄ isomer	82	198	C ₅ H ₉ -benzene isomer
62	167	C ₄ -alkyl benzene isomer	82A	198	C ₆ -alkyl benzene isomer
62A	168	C ₁₀ H ₁₈ isomer	83	199	C ₁₃ H ₂₆ isomer (tent.)
62B	168	C ₁₁ H ₂₄ isomer	85	203	C ₁₃ H ₂₆ isomer
63	169	C ₄ -alkyl benzene isomer	86	204	n-tridecane
63A	170	C ₁₁ H ₂₂ isomer	86A	205	β-methylnaphthalene
64	170	C ₄ -alkyl benzene isomer	86B	206	C ₁₃ H ₂₆ isomer
65	171	C ₄ H ₇ -benzene + C ₁₁ H ₂₂ isomers	87	207	α-methylnaphthalene
65A	171	C ₄ -alkyl benzene isomer	88	211	sat. hydrocarbon (tent.)
65B	172	C ₁₁ H ₂₂ isomer	89	213	C ₁₄ H ₃₀ isomer
66	173	n-undecane	90	214	alkyl butyrate
66A	173	C ₅ -alkyl benzene isomer	90A	215	biphenyl
67	176	C ₄ -alkyl benzene isomer	90B	216	C ₁₄ H ₂₈ isomer
67A	174	C ₅ -alkyl benzene isomer	90C	217	diphenyl ether or C ₁₂ H ₁₀ O isomer
67B	175	C ₁₁ H ₂₂ isomer	91	218	n-tetradecane
68	176	tetramethylbenzene isomer	91A	220	dimethylnaphthalene isomer
69	177	C ₄ -alkyl benzene isomer	92	223	dimethylnaphthalene isomer
69A	178	C ₂ -alkyl phenol isomer	93	226	C ₁₅ H ₃₂ isomer (tent.)
70	179	C ₅ -alkyl benzene isomer	93A	227	C ₁₅ H ₃₀ isomer
71	180	C ₅ -alkyl benzene + C ₄ H ₇ -benzene isomers	94	230	n-pentadecane

(continued)

Table C-2. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
95	233	unknown	100	240	<u>n</u> -heptadecane
96	239	diethyl phthalate	101	240	unsat. hydrocarbon
99	240	unsat. hydrocarbon	102	240	sat. hydrocarbon

Table C-3. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED
IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L5).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	14	68	3-methylpentane
4	52	<u>n</u> -propane (tent.)	15	70	hexafluorobenzene (e\$)
4A	53	butene isomer	16	71	<u>n</u> -hexane
5	53	<u>n</u> -butane	16A	72	chloroform
5A	54	butene (tent.)	17	75	perfluorotoluene (e\$)
6	55	acetaldehyde	18	76	methylcyclopentane
7	57	isopentane	18A	77	C ₆ H ₁₀ isomer
8	58	acetone	18B	78	benzene
9	59	<u>n</u> -pentane	18C	79	carbon tetrachloride
9A	60	diethyl ether	18D	80	cyclohexane
10	61	vinylidene chloride	19	103	toluene
10A	61	methylene chloride	19A	107	acetic acid (tent.)
12	63	CS ₂	20	145	phenol
13	66	2-methylpentane	20A	146	C ₁₁ H ₂₄ isomer
13A	68	<u>n</u> -butanal			

Table C-4. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L5).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	26	132	C ₉ H ₂₀ isomer
2A	54	propane	26A	133	C ₇ H ₁₄ O isomer (tent.)
2B	55	butane	26B	133	styrene
2C	55	acetaldehyde	27	134	<i>o</i> -xylene
2D	60	dimethyl ether	27A	135	C ₉ H ₁₈ isomer
2E	60	isopentane	28	137	<i>n</i> -nonane
3	61	acetone	28A	140	C ₉ H ₁₈ isomer
3A	65	vinylidene chloride	29	140	isopropylbenzene
4	66	dichloromethane	30	142	C ₁₀ H ₂₂ isomer
6	74	2-methylpentane	31	143	C ₁₀ H ₂₂ isomer
6A	75	C ₆ H ₁₂ isomer	31A	144	C ₃ -alkyl cyclohexane isomer
6B	76	3-methylpentane	31B	145	C ₁₀ H ₂₂ isomer
7	78	hexafluorobenzene (e§)	32	145	benzaldehyde
8	79	<i>n</i> -hexane	33	146	<i>n</i> -propylbenzene + C ₁₀ H ₂₀ isomer
8A	80	chloroform	34	147	ethyltoluene isomer
8B	81	C ₄ H ₈ O isomer	34A	148	C ₁₀ H ₂₂ isomer + phenol
8C	82	ethyl acetate	35	149	1,3,5-trimethylbenzene + C ₁₁ H ₂₄ isomer
9	83	perfluorotoluene (e§)	36	150	C ₁₀ H ₂₂ isomer
9A	84	methylcyclopentane	36A	151	<i>o</i> -ethyltoluene
9B	86	1,1,1-trichloroethane	37	151	C ₁₀ H ₂₂ isomer
9C	88	C ₆ H ₁₀ isomer	37A	152	C ₁₀ H ₂₀ isomer
10	89	benzene	38	153	<i>n</i> -octanal
10A	90	carbon tetrachloride	39	153	1,2,4-trimethylbenzene
10B	91	acetic acid (tent.)	39A	154	C ₁₀ H ₂₀ isomer
11	91	C ₇ H ₁₆ isomer	40	155	<i>n</i> -decane
12	93	C ₇ H ₁₆ isomer	41	156	dichlorobenzene isomer
13	95	C ₇ H ₁₄ isomer	41A	157	C ₄ -alkyl benzene isomer
13A	96	trichloroethylene (tent.)	41B	158	C ₁₁ H ₂₂ + C ₄ -alkyl benzene isomers
14	96	C ₈ H ₁₈ isomer	42	159	1,2,3-trimethylbenzene
15	98	<i>n</i> -heptane	43	159	C ₁₁ H ₂₄ isomer
16	102	methylcyclohexane	43A	160	C ₈ H ₁₆ O isomer
17	104	C ₈ H ₁₈ + C ₇ H ₁₄ O isomer	44	160	C ₁₁ H ₂₄ isomer
18	109	toluene	44A	161	indan
19	110	C ₈ H ₁₈ isomer	44B	162	C ₁₁ H ₂₂ isomer
20	112	C ₈ H ₁₈ isomer	45	162	C ₄ -alkyl cyclohexane isomer
20A	113	C ₈ H ₁₆ isomer	46	163	C ₄ -alkyl benzene isomer
20B	114	hexanal (tent.)	47	164	acetophenone
20C	115	C ₈ H ₁₆ isomer	47A	165	C ₄ -alkyl benzene isomer
21	117	<i>n</i> -octane	48	165	C ₁₂ H ₂₄ isomer
22	118	tetrachloroethylene	49	166	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers
22A	122	C ₈ H ₁₆ isomer	50	168	C ₄ -alkyl benzene isomer
22B	123	C ₉ H ₂₀ isomer	50A	169	C ₁₁ H ₂₂ isomer
23	125	C ₉ H ₂₀ isomer (tent.)			
24	128	ethylbenzene			
25	130	xylene isomer			
25A	130	C ₉ H ₂₀ isomer			

(continued)

Table C-4. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
51	169	C ₄ -alkyl benzene isomer	58A	189	C ₅ -alkyl benzene isomer
52	170	n-nonanal	58B	190	C ₁₃ H ₂₆ isomer
52A	171	C ₁₁ H ₂₂ isomer	58C	190	C ₃ -alkyl phenol isomer
53	172	n-undecane	58D	191	C ₁₃ H ₂₈ isomer
53A	173	C ₄ -alkyl benzene isomer	59A	195	unsaturated hydrocarbon
53B	174	C ₁₁ H ₂₂ isomer	59B	199	saturated hydrocarbon
54	175	C ₄ -alkyl benzene isomer	59C	201	C ₁₁ H ₂₂ O isomer
55	177	C ₂ -alkyl phenol isomer	59D	201	n-undecanal (tent.)
55A	178	C ₅ -alkyl benzene isomer	60	202	n-tridecane
55B	178	C ₁₂ H ₂₄ isomer	60A	203	β-methylnaphthalene
55C	179	C ₄ H ₇ -benzene isomer	61	205	α-methylnaphthalene
55D	179	C ₅ -alkyl cyclohexane isomer	62	211	alkyl butyrate (tent.)
56	180	C ₂ -alkyl phenol isomer	63	212	alkyl butyrate (tent.)
56A	181	C ₄ H ₇ -benzene isomer	64	213	biphenyl
56B	181	C ₄ -alkyl benzene isomer	64A	215	C ₁₄ H ₂₈ isomer (tent.)
56C	183	C ₅ -alkyl benzene isomer	65	216	n-tetradecane + diphenyl ether (tent.)
56D	184	C ₁₂ H ₂₆ + C ₅ -alkyl benzene isomers	65A	220	C ₂ -alkyl naphthalene (tent.)
56E	185	C ₃ -alkyl phenol isomer	66	225	saturated hydrocarbon
57	186	naphthalene	66A	228	C ₁₅ H ₃₀ isomer (tent.)
57A	187	n-decanal	67	229	n-pentadecane
57B	187	C ₁₂ H ₂₄ isomer	68	231	unknown
57C	188	C ₅ -alkyl benzene isomer	71	240	C ₁₇ H ₃₆ isomer
58	188	n-dodecane	72	240	n-heptadecane

Table C-5. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L6).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	11A	66	C ₅ H ₁₀ isomer (tent.)
3	53	propane	12	67	2-methylpentane
3A	53	C ₄ H ₈ isomer	13	70	3-methylpentane
4	54	<u>n</u> -butane	14	71	hexafluorobenzene (e ₂)
4A	55	butene isomer	15	72	<u>n</u> -hexane
4B	55	acetaldehyde	15A	73	chloroform
5	57	isopentane	16	76	perfluorobenzene (e ₂)
7	58	acetone	17	77	methylcyclopentane
8	59	<u>n</u> -pentane	17A	79	1,1,1-trichloroethane (tent.)
8A	59	C ₅ H ₁₀ isomer	17B	82	benzene
8B	60	vinylidene chloride	17C	84	cyclohexane
9	61	methylene chloride	17E	96	methylcyclohexane
11	63	CS ₂	18	104	toluene

Table C-6. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 1, P2/L6).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	28C	115	C ₈ H ₁₆ isomer
2A	53	propane	29	115	C ₈ H ₁₆ isomer
2B	54	C ₄ H ₈ isomer	30	116	n-octane
2C	54	n-butane	30A	117	C ₈ H ₁₆ isomer
2D	56	acetaldehyde	31	118	tetrachloroethylene
2E	59	dimethyl ether	32	120	C ₉ H ₂₀ isomer
3	60	acetone	33	121	C ₉ H ₂₀ isomer
3B	63	diethyl ether	34	123	C ₉ H ₂₀ isomer
4	64	vinylidene chloride	34A	123	C ₉ H ₁₈ isomer
5	65	dichloromethane	35	124	C ₉ H ₂₀ isomer
6A	70	C ₄ H ₆ O isomer (tent.)	35A	125	C ₉ H ₁₈ isomer
7	71	2-methylpentane	36	128	ethylbenzene
8	74	3-methylpentane	36A	128	C ₉ H ₁₈ isomer
8A	74	n-butanal	37	129	xylene isomer
8B	75	C ₆ H ₁₂ isomer	37A	130	C ₉ H ₂₀ isomer
9	75	hexafluorobenzene (eS)	38	131	C ₉ H ₂₀ isomer
10	76	n-hexane	38A	132	C ₇ H ₁₄ O isomer (tent.)
10A	77	chloroform	39	133	styrene
10B	78	methyl ethyl ketone	40	134	o-xylene
11	79	ethyl acetate	40A	135	C ₉ H ₁₈ isomer
11A	80	C ₆ H ₁₂ isomer	41	136	n-nonane
12	81	perfluorotoluene (eS)	41A	138	C ₁₀ H ₂₀ isomer
13	82	methylcyclopentane	42	139	C ₉ H ₁₈ isomer
14	83	1,1,1-trichloroethane	43	140	isopropylbenzene + C ₁₀ H ₂₂ isomer
15	86	benzene	44	141	C ₉ H ₁₆ isomer
15A	88	cyclohexane	44A	142	C ₇ H ₁₄ O isomer (tent.)
16	89	2-methylhexane	45	143	C ₁₀ H ₂₂ isomer
16A	90	2,3-dimethylpentane	45A	144	C ₃ -alkyl cyclohexane isomer
17	91	3-methylhexane	45B	145	C ₁₀ H ₂₀ isomer
18	93	C ₇ H ₁₄ isomer	46	145	benzaldehyde
19	94	trichloroethylene (tent.) + C ₈ H ₁₈ isomer	47	146	n-propylbenzene
19A	95	acetic acid	48	147	ethyltoluene isomer
20	96	n-heptane	48A	148	C ₁₀ H ₂₂ isomer
20A	97	C ₇ H ₁₄ isomer	49	149	1,3,5-trimethylbenzene
21	101	methylcyclohexane	49A	150	C ₁₀ H ₂₀ isomer
22	103	C ₈ H ₁₈ isomer	50	150	C ₁₀ H ₂₂ isomer
23	105	C ₈ H ₁₆ isomer	51	151	o-ethyltoluene
24	107	C ₈ H ₁₈ isomer	52	152	C ₁₀ H ₂₀ isomer
25	108	toluene	52A	153	C ₁₀ H ₂₀ isomer
26	109	C ₈ H ₁₈ isomer	53	153	n-octanal + methylstyrene isomer (tent.)
26A	110	C ₈ H ₁₆ isomer	54	154	1,2,4-trimethylbenzene
27	111	C ₈ H ₁₈ isomer	54A	153	C ₁₀ H ₂₀ isomer
28	113	C ₈ H ₁₆ isomer	55	155	n-decane
28A	114	C ₈ H ₁₈ isomer	55A	156	C ₁₀ H ₂₀ isomer
28B	114	C ₆ H ₁₂ O isomer			

(continued)

Table C-6. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
56	156	C ₄ -alkyl benzene isomer	75	179	C ₅ -alkyl cyclohexane isomer
57	158	C ₁₁ H ₂₄ isomer	75A	180	C ₁₂ H ₂₄ isomer
57A	158	C ₄ -alkyl benzene isomer	75B	180	C ₅ -alkyl benzene isomer
58	159	1,2,3-trimethylbenzene	76	181	C ₄ H ₇ -benzene isomer
59	160	C ₁₁ H ₂₄ isomer	76A	181	C ₄ -alkyl benzene isomer
60	161	C ₁₁ H ₂₄ + dichlorobenzene isomers (tent.)	76B	182	C ₅ -alkyl benzene isomer
60A	161	indan + C ₁₁ H ₂₂ isomer	77	183	C ₁₂ H ₂₆ isomer
61	162	C ₄ -alkyl cyclohexane isomer	77A	184	C ₁₂ H ₂₆ isomer
61A	163	C ₄ -alkyl benzene isomer	77B	184	C ₅ -alkyl benzene isomer
62	163	C ₄ -alkyl benzene isomer	78	186	naphthalene
62A	163	C ₁₁ H ₂₄ isomer	78A	187	C ₁₂ H ₂₄ isomer
63	164	C ₄ -alkyl benzene isomer + acetophenone	79	188	3-dodecane
63A	164	n-butylbenzene	79A	189	C ₅ -alkyl benzene isomer
64	165	C ₁₁ H ₂₂ isomer	79B	195	C ₁₂ H ₂₄ isomer
65	165	C ₁₁ H ₂₄ isomer	80	199	sat. hydrocarbon
66	166	C ₄ -alkyl benzene isomer	80A	202	C ₁₃ H ₂₆ isomer
66A	166	C ₁₁ H ₂₂ isomer	81	203	n-tridecane
66B	167	C ₁₀ H ₁₈ isomer	81A	204	β-methylnaphthalene
67	167	C ₁₁ H ₂₄ isomer	81B	204	C ₁₃ H ₂₆ isomer
67A	168	C ₄ -alkyl benzene isomer	82	206	α-methylnaphthalene
67B	168	C ₁₁ H ₂₂ isomer	82A	208	C ₁₃ H ₂₆ isomer
68	169	C ₄ -alkyl benzene isomer	83	211	C ₇ -alkyl cyclohexane or C ₁₃ H ₂₆ isomer
69	170	C ₁₁ H ₂₂ isomer	84	212	alkyl butyrate
70	171	n-nonanal	85	213	alkyl butyrate
71	172	n-undecane	86	217	n-tetradecane
71A	173	C ₄ -alkyl benzene isomer	86A	219	C ₂ -alkyl naphthalene isomer
72	174	C ₁₁ H ₂₂ isomer	86B	221	C ₂ -alkyl naphthalene isomer
73	176	C ₄ -alkyl benzene + C ₁₂ H ₂₆ isomers	86C	225	C ₁₅ H ₃₀ isomer
74	177	C ₁₂ H ₂₄ isomer	88	229	n-pentadecane
74A	178	C ₅ -alkyl benzene + C ₂ -alkyl phenol isomers (tent.)	89	232	unknown
74B	179	C ₄ -benzene + C ₅ -alkyl benzene isomers	89A	237	C ₁₆ H ₃₂ isomer
			90	238	diethyl phthalate
			91A	240	n-hexadecane

Table C-7. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 2, P2/L3).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	24	86	2,3-dimethylpentane
3A	53	C ₄ H ₈ isomer	24A	86	alkyl ether (tent.)
4	54	acetaldehyde	25	87	3-methylhexane
4A	54	n-butane	26	88	3-pentanone
4B	55	methyl formate (tent.)	26A	89	C ₇ H ₁₄ isomer
5	58	isopentane	27	90	1,1,1-trichloroethylene
5A	58	dimethyl ether (tent.)	27A	91	C ₇ H ₁₄ isomer
6	59	acetone	28	92	n-heptane
6A	59	furan (tent.)	28A	92	n-propyl acetate
6B	60	C ₅ H ₁₀ isomer	28B	93	C ₇ H ₁₄ isomer
7	60	n-pentane	29	94	C ₇ H ₁₄ isomer
8	61	C ₅ H ₁₀ isomer	30	97	methylcyclohexane
8A	62	isopropanol (tent.)	30A	98	4-methyl-2-pentanone
8B	62	C ₅ H ₁₀ isomer	31	98	C ₈ H ₁₈ isomer
8C	62	methylene chloride	32	99	C ₈ H ₁₈ isomer
9	63	methyl acetate	33	101	C ₈ H ₁₆ isomer
9B	64	carbon disulfide	33A	102	2-ethylbutanal
10	66	2-methylpropanal	34	103	C ₈ H ₁₈ isomer
10A	67	C ₆ H ₁₂ isomer	34A	104	C ₈ H ₁₆ isomer
10B	68	C ₄ H ₆ O isomer	35	104	toluene
11	68	2-methylpentane	36	106	C ₈ H ₁₈ isomer
11A	69	methyl isopropyl ketone (tent.)	36A	107	alkyl ether (tent.)
12	70	3-methylpentane	37	107	C ₈ H ₁₈ isomer
13	71	methyl ethyl ketone	37A	109	dimethylcyclohexane isomer
13A	71	C ₆ H ₁₂ isomer	38	109	C ₈ H ₁₈ isomer (tent.)
14	72	hexafluorobenzene (e3)	38A	110	1,2-dibromoethane (tent.)
15	73	n-hexane	38B	111	alcohol isomer (tent.)
15A	73	isopropyl ether	39	112	C ₈ H ₁₆ isomer
15B	74	chloroform	40	113	n-octane
15C	74	C ₆ H ₁₂ isomer	40A	113	n-butyl acetate
16	75	ethyl acetate	41	114	tetrachloroethylene
16A	75	C ₆ H ₁₂ isomer	41A	115	C ₈ H ₁₆ isomer
16B	76	C ₆ H ₁₂ isomer	42	117	C ₉ H ₂₀ isomer
17	77	perfluorotoluene (e3)	43	118	C ₉ H ₂₀ isomer
18	78	methylcyclopentane	44	119	C ₉ H ₂₀ isomer
18A	79	1,2-dichloroethane (tent.)	44A	120	C ₈ H ₁₆ isomer
18B	79	1,1,1-trichloroethane	44B	120	C ₉ H ₁₈ isomer
19	80	unknown	45	121	C ₉ H ₂₀ isomer
19A	82	C ₆ H ₁₀ isomer	45A	122	C ₉ H ₁₈ isomer
20	82	isopropyl acetate	45B	123	C ₉ H ₁₈ isomer
20A	83	benzene	46	124	ethylbenzene
21	83	carbon tetrachloride	46A	124	C ₉ H ₁₈ isomer
22	84	isopropenyl acetate + hexane	47	126	xylene isomer
23	85	2-methylhexane	47A	126	C ₉ H ₂₀ isomer
			48	128	C ₉ H ₂₀ isomer
			49	129	C ₇ H ₁₄ O isomer (tent.)

(continued)

Table C-7. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
50	130	styrene	72	156	1,2,3-trimethylbenzene
50A	130	heptanal	73	156	C ₁₁ H ₂₄ isomer
51	131	<i>o</i> -xylene	74	157	dichlorobenzene + C ₁₁ H ₂₄ isomers
52	132	C ₉ H ₁₈ isomer	74A	158	indan + C ₁₀ H ₂₀ isomer
53	133	cyclohexyl acetate or C ₆ H ₁₁ acetate isomer	74B	158	C ₁₁ H ₂₄ isomer
54	133	<i>n</i> -nonane	75	159	C ₄ -alkyl cyclohexane isomer
54A	134	C ₁₀ H ₂₀ isomer	75A	159	C ₄ -alkyl benzene isomer
55	136	C ₉ H ₁₈ isomer	76	160	propyltoluene isomer
55A	137	C ₁₀ H ₂₂ isomer	77	161	C ₄ -alkyl benzene isomer
56	137	isopropylbenzene	78	162	C ₁₁ H ₂₄ isomer
56A	137	C ₁₀ H ₂₂ isomer	78A	162	C ₁₁ H ₂₂ isomer
56B	138	C ₁₀ H ₂₀ isomer	79	163	C ₁₁ H ₂₄ isomer
57	139	C ₉ H ₁₆ + C ₁₀ H ₂₂ isomer	80	163	C ₄ -alkyl benzene isomer
57A	140	C ₁₀ H ₂₀ isomer	80A	164	C ₁₀ H ₁₈ isomer
58	140	C ₃ -alkyl cyclohexane + C ₁₀ H ₂₂ isomers	81	164	C ₁₁ H ₂₄ isomer
58A	141	C ₁₀ H ₂₂ isomer	81A	165	C ₄ -alkyl benzene isomer
59	141	C ₁₀ H ₁₆ + C ₈ H ₁₆ O isomers	81B	166	C ₄ H ₇ -benzene + C ₁₁ H ₂₂ isomers
59A	142	C ₁₀ H ₂₂ isomer	82	167	C ₄ -alkyl benzene isomer
60	142	benzaldehyde	83	167	C ₄ H ₇ -benzene + C ₁₁ H ₂₂ isomers
60A	142	C ₁₀ H ₂₀ isomer	83A	168	C ₁₁ H ₂₂ isomer
61	142	<i>n</i> -propylbenzene	84	169	<i>n</i> -undecane
61A	143	C ₁₀ H ₂₀ isomer	85	170	C ₄ -alkyl benzene isomer
62	144	ethyltoluene isomer	85A	170	C ₁₁ H ₂₂ isomer
62A	145	C ₁₀ H ₂₂ isomer	85B	171	C ₄ -alkyl benzene isomer
62B	145	phenol (cont.)	85C	171	C ₁₂ H ₂₆ isomer
63	146	1,3,5-trimethylbenzene	86	172	tetramethylbenzene + C ₁₂ H ₂₆ isomers
63A	146	C ₁₀ H ₂₀ isomer	87	173	C ₄ -alkyl benzene isomer
64	147	C ₁₀ H ₂₂ isomer	87A	174	C ₁₁ H ₂₀ isomer
65	148	<i>o</i> -ethyltoluene	88	174	C ₁₂ H ₂₆ + C ₂ -alkyl phenol isomers
65A	148	C ₁₀ H ₁₈ + C ₁₁ H ₂₄ isomers	89	175	C ₅ -alkyl benzene isomer
66	149	C ₁₀ H ₂₀ isomer	89A	175	C ₁₂ H ₂₄ isomer
66A	149	C ₁₀ H ₁₈ isomer	90	176	C ₅ -alkyl benzene + C ₄ H ₇ -benzene isomers
67	150	C ₁₀ H ₂₂ isomer	91	176	C ₅ -alkyl cyclohexane isomer
67A	150	C ₃ H ₅ -benzene isomer	91A	177	C ₁₁ H ₂₀ + C ₁₂ H ₂₄ isomers
68	151	1,2,4-trimethylbenzene	91B	177	C ₂ -alkyl phenol isomer
68A	152	C ₁₀ H ₂₀ isomer	92	177	C ₄ H ₇ -benzene + C ₅ -alkyl benzene isomers
69	152	<i>n</i> -decane	93	178	C ₄ -alkyl benzene isomer
69A	153	dichlorobenzene isomer	93A	178	C ₁₂ H ₂₆ isomer
70	153	C ₁₀ H ₂₀ isomer + isobutylbenzene	94	179	C ₅ -alkyl benzene isomer
70A	154	sec-butylbenzene	95	180	1,2,3,4-tetrahydronaphthalene + C ₅ -alkyl benzene isomer
70B	155	C ₁₁ H ₂₂ isomer			
71	155	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers			

(continued)

Table C-7. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
95A	180	C ₁₂ H ₂₄ isomer	110A	207	C ₆ -alkyl benzene isomer
96	181	C ₅ -alkyl benzene isomer	110B	208	C ₁₃ H ₂₆ isomer
96A	182	C ₁₂ H ₂₄ isomer	111	209	C ₁₄ H ₃₀ isomer
96B	182	C ₆ -alkyl benzene isomer	112	210	alkyl butyrate
96C	183	C ₅ H ₉ -benzene + C ₁₂ H ₂₄ isomers	113	211	C ₁₅ H ₃₂ isomer
97	183	naphthalene	113A	211	biphenyl
97A	184	C ₅ -alkyl benzene isomer	113B	212	C ₁₄ H ₂₈ isomer
97B	184	C ₅ -alkyl benzene + C ₁₂ H ₂₄ isomers	114	213	n-tetradecane
98	185	n-dodecane	114A	214	C ₂ -alkyl naphthalene isomer
99	186	C ₅ -alkyl benzene + C ₁₂ H ₂₄ isomers	115	216	C ₂ -alkyl naphthalene isomer
100	187	C ₁₃ H ₂₈ isomer	115A	217	C ₁₅ H ₃₀ isomer
101	188	C ₆ -alkyl benzene isomer	116	218	dimethylnaphthalene isomer
101A	189	C ₁₃ H ₂₈ isomer	116A	219	C ₁₅ H ₃₀ isomer
101B	190	C ₁₃ H ₂₆ isomer	116B	219	C ₁₅ H ₃₂ isomer
102	190	C ₆ -alkyl benzene isomer	117	220	C ₂ -alkyl naphthalene isomer
102A	191	C ₁₃ H ₂₆ isomer	118	222	C ₁₆ H ₃₄ isomer
103	192	C ₆ -alkyl cyclohexane isomer	119	224	C ₁₃ H ₂₆ O isomer (tent.)
103A	193	C ₅ -alkyl benzene isomer	120	225	C ₁₅ H ₃₀ isomer
104	193	C ₁₃ H ₂₈ isomer	121	226	n-pentadecane
104A	193	C ₅ H ₉ -benzene isomer	122	228	unknown
105	194	C ₆ -alkyl benzene isomer	122A	233	C ₁₆ H ₃₄ + C ₃ -alkyl naphthalene isomers
106	195	C ₁₃ H ₂₈ isomer	122B	234	unsat. hydrocarbon
107	196	C ₁₄ H ₃₀ isomer	123	235	diethyl phthalate (BKG)
107A	198	C ₁₃ H ₂₆ isomer	123A	237	C ₁₄ H ₂₈ O isomer
108	200	n-tridecane	123B	238	C ₁₆ H ₃₂ isomer
108A	200	β-methylnaphthalene	125	240	unknown
108B	202	C ₅ -alkyl benzene isomer	127	240	sat. hydrocarbon
109	203	α-methylnaphthalene	128	240	C ₁₅ H ₃₀ O isomer
109A	204	C ₁₄ H ₂₈ isomer	128A	240	C ₁₇ H ₃₄ isomer
109B	206	C ₁₄ H ₂₈ isomer	129	240	n-heptadecane
110	207	C ₁₄ H ₃₀ isomer	130	240	sat. hydrocarbon
			131	240	n-octadecane

Table C-8. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 2, P2/L4).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	20A	89	C ₇ H ₁₆ isomer
2A	53	C ₄ H ₈ isomer	21	89	trichloroethylene
2B	53	n-butane	21A	90	C ₇ H ₁₄ isomer
2C	54	acetaldehyde (tent.)	22	91	n-heptane
2D	54	C ₄ H ₈ isomer	22A	92	C ₇ H ₁₄ isomer
2E	56	C ₅ H ₁₀ isomer	22B	93	n-propyl acetate
3	58	isopentane	23	94	C ₇ H ₁₄ isomer
4	59	acetone	23A	94	C ₇ H ₁₂ isomer
4A	59	C ₅ H ₁₀ isomer	24	96	methylcyclohexane
5	60	n-pentane	24A	97	4-methyl-2-pentanone
5A	60	C ₅ H ₁₀ isomer	24B	98	C ₈ H ₁₈ isomer
5B	61	isopropanol	24C	98	dimethyl disulfide
5C	62	dichloromethane + C ₅ H ₁₀ isomer	25	98	C ₈ H ₁₈ isomer
6	63	methyl acetate	26	100	C ₈ H ₁₆ isomer
6A	64	C ₅ H ₈ isomer	27	102	C ₈ H ₁₈ -- C ₇ H ₁₂ isomers (tent.)
6B	64	CS ₂	28	104	toluene
6C	66	2-methylpropanal	29	105	C ₈ H ₁₈ isomer
6D	67	C ₅ H ₈ isomer	30	107	C ₈ H ₁₈ isomer
7	68	2-methylpentane	31	108	C ₈ H ₁₆ isomer
8	70	3-methylpentane	32	109	C ₈ H ₁₈ isomer
8A	71	C ₆ H ₁₂ isomer + methyl ethyl ketone (tent.)	32A	110	C ₈ H ₁₆ isomer
9	72	hexafluorobenzene (e§)	32B	110	1,2-dibromoethane (tent.)
10	73	n-hexane	33	111	C ₈ H ₁₆ isomer
10A	73	isopropyl ether	34	112	n-octane
11	74	chloroform + C ₆ H ₁₂ isomer	34A	113	C ₈ H ₁₆ isomer
12	75	C ₆ H ₁₂ isomer	35	114	tetrachloroethylene
12A	75	ethyl acetate (tent.)	35A	114	C ₈ H ₁₆ isomer
12B	76	C ₆ H ₁₂ isomer	36	116	dimethylpentanal or C ₇ H ₁₄ O isomer
13	76	perfluorotoluene (e§)	37	117	C ₉ H ₂₀ isomer
14	77	C ₆ H ₁₂ isomer	37A	118	C ₈ H ₁₄ isomer (tent.)
14A	78	1,1,1-trichloroethane	38	118	C ₉ H ₂₀ isomer
15	80	1-chlorobutane	39	119	4-vinylcyclohexene
16	81	unknown	39A	119	C ₈ H ₁₆ isomer
16A	82	C ₆ H ₁₀ isomer	39B	120	C ₉ H ₁₈ isomer
17	82	benzene	40	120	C ₉ H ₂₀ isomer + ethylcyclohexane
17A	83	isopropyl acetate (tent.)	41	121	trimethylcyclohexane isomer
17B	83	carbon tetrachloride	41A	128	C ₉ H ₁₈ isomer
17C	84	cyclohexane	41B	123	C ₉ H ₁₆ isomer
18	84	2-methylhexane	41C	123	C ₉ H ₁₈ isomer
18A	85	2,3-dimethylpentane	42	124	ethylbenzene
19	86	3-methylhexane	43	124	C ₉ H ₁₈ isomer
19A	87	C ₆ H ₁₀ isomer	43A	125	C ₉ H ₂₀ isomer
19B	88	C ₅ H ₁₀ O isomer	44	125	xylene isomer
19C	88	C ₇ H ₁₄ isomer	44A	126	C ₉ H ₂₀ isomer
20	88	dichloropropene			

(continued)

Table C-8. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
45	127	C ₉ H ₂₀ isomer	67	155	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers
46	128	C ₇ H ₁₄ O + C ₉ H ₁₈ isomers	68	156	1,2,3-trimethylbenzene
46A	129	C ₉ H ₁₈ isomer	69	156	C ₁₁ H ₂₄ isomer
47	129	styrene	70	157	C ₁₁ H ₂₄ isomer + o-dichlorobenzene
47A	129	tetrahydroindene or C ₉ H ₁₂ isomer	70A	158	indan
48	130	o-xylene	71	159	C ₄ -alkyl cyclohexane isomer
48A	130	C ₉ H ₁₈ isomer	71A	160	C ₁₁ H ₂₂ + C ₄ -alkyl benzene isomers
49	131	methylcyclohexane isomer	72	160	C ₄ -alkyl benzene isomer
50	133	n-nonane	73	161	C ₄ -alkyl benzene isomer + n-butylbenzene
50A	134	anisole	74	162	C ₁₁ H ₂₄ isomer
50B	135	C ₁₀ H ₂₀ isomer	75	162	C ₁₁ H ₂₂ isomer
50C	135	C ₁₀ H ₂₂ isomer	75A	163	C ₄ -alkyl benzene isomer
51	136	C ₃ -alkyl cyclohexane isomer	76	163	C ₁₁ H ₂₂ isomer
51A	136	C ₉ H ₁₂ isomer	76A	163	C ₄ -alkyl benzene isomer
52	137	isopropylbenzene + C ₁₀ H ₂₂ isomer	76B	164	C ₁₀ H ₁₈ isomer
52A	138	C ₁₀ H ₂₀ isomer	77	164	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers
53	138	C ₉ H ₁₆ isomer	78	165	C ₄ -alkyl benzene isomer
53A	139	C ₁₀ H ₂₂ isomer	78A	165	C ₁₁ H ₂₀ isomer
53B	140	C ₁₀ H ₂₀ isomer	78B	165	C ₁₁ H ₂₂ isomer
54	140	propylcyclohexane	79	166	C ₄ -alkyl benzene isomer
54A	141	C ₁₀ H ₂₂ isomer	79A	166	C ₁₂ H ₂₂ isomer
55	141	C ₁₀ H ₁₆ isomer	80	167	C ₁₁ H ₂₂ isomer
55A	142	C ₁₀ H ₂₂ isomer	81	168	C ₁₁ H ₂₂ isomer
56	142	C ₁₀ H ₂₀ isomer + benzaldehyde	81A	168	C ₁₂ H ₂₄ isomer
57	143	n-propylbenzene	82	169	n-undecane
57A	143	C ₁₀ H ₂₀ isomer	82A	170	C ₄ -alkyl benzene isomer
58	144	ethyltoluene isomer	83	170	C ₁₁ H ₂₂ isomer
58A	145	C ₁₀ H ₂₂ isomer	83A	171	C ₁₂ H ₂₄ isomer
59	145	1,3,5-trimethylbenzene + C ₁₀ H ₂₂ isomer	83B	171	C ₁₂ H ₂₆ isomer
59A	146	C ₁₀ H ₂₀ isomer	83C	171	C ₄ -alkyl benzene isomer
60	147	C ₁₀ H ₂₂ isomer	84	172	C ₁₂ H ₂₆ isomer
61	148	o-ethyltoluene	84A	173	C ₁₁ H ₂₀ isomer
62	148	C ₁₀ H ₁₈ isomer	85	174	C ₁₂ H ₂₆ isomer
63	149	C ₁₀ H ₂₀ isomer	85A	174	C ₂ -alkyl phenol isomer
63A	150	C ₃ H ₅ -benzene isomer	86	175	C ₅ -alkyl benzene isomer
64	150	1,2,4-trimethylbenzene	86A	175	C ₁₂ H ₂₄ isomer
64A	151	C ₁₀ H ₂₀ isomer	86B	176	C ₅ -alkyl benzene + C ₄ H ₇ - benzene isomers
65	152	n-decane	87	177	C ₅ -alkyl cyclohexane isomer
65A	153	dichlorobenzene isomer (tent.)	87A	177	C ₁₁ H ₂₀ isomer
66	153	C ₁₀ H ₂₀ isomer			
66A	154	C ₄ -alkyl benzene isomer			
66B	154	C ₁₁ H ₂₂ isomer (tent.)			

(continued)

Table C-8. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
87B	177	C ₅ -alkyl benzene + C ₂ -alkyl phenol isomer	105A	203	C ₆ H ₁₁ -benzene isomer (tent.)
87C	178	C ₄ H ₇ -benzene + C ₁₂ H ₂₄ isomers	105B	205	C ₇ -alkyl benzene isomer
88	178	C ₁₂ H ₂₆ + tetramethylbenzene isomers	105C	206	C ₁₄ H ₂₈ isomer
89	179	C ₅ -alkyl benzene isomer	106	207	C ₇ -alkyl cyclohexane or C ₁₃ H ₂₆ isomer
90	180	1,2,3,4-tetrahydronaphthalene + C ₅ -alkyl benzene isomer	106A	208	C ₁₅ H ₃₂ isomer
90A	180	C ₆ -alkyl benzene isomer	107	209	C ₁₀ H ₁₀ O ketone isomer
91	181	C ₅ -alkyl benzene + C ₁₂ H ₂₆ isomers	107A	210	C ₁₅ H ₃₀ isomer
91A	182	C ₁₂ H ₂₄ isomer	108	211	biphenyl
92	183	naphthalene	108A	211	C ₁₄ H ₂₈ isomer
92A	184	C ₁₂ H ₂₄ isomer	109	213	n-tetradecane + diphenyl ether
92B	184	C ₅ -alkyl benzene isomer	110	215	dimethylnaphthalene isomer
93	185	n-dodecane	111	217	dimethylnaphthalene isomer
94	186	C ₅ -alkyl benzene isomer	111A	218	C ₁₅ H ₃₀ isomer
95	187	C ₁₃ H ₂₈ isomer	112	220	C ₁₅ H ₃₂ isomer
96	188	C ₆ -alkyl benzene isomer	113	222	C ₁₆ H ₃₄ isomer
96A	190	C ₆ -alkyl benzene isomer	113A	224	C ₁₅ H ₃₀ isomer
97	191	C ₁₃ H ₂₆ isomer	113B	225	C ₁₅ H ₃₀ isomer
98	192	C ₆ -alkyl cyclohexane isomer	114	226	n-pentadecane
98A	192	C ₁₃ H ₂₆ isomer	115	228	unknown
99	193	C ₁₃ H ₂₈ isomer	115A	231	C ₁₅ H ₃₀ isomer
100	194	C ₆ -alkyl benzene isomer	115B	232	C ₃ -alkyl naphthalene isomer
100A	195	C ₁₃ H ₂₈ isomer	116	235	diethyl phthalate
101	196	C ₁₄ H ₃₀ isomer	117	237	C ₁₄ H ₂₈ O isomer
101A	197	C ₁₁ H ₂₂ O isomer	117A	237	C ₁₆ H ₃₂ isomer
102	198	C ₁₃ H ₂₆ isomer	118A	239	n-hexadecane
103	199	n-tridecane	119	240	unknown
103A	200	β-methylnaphthalene	119A	240	benzophenone
104	201	C ₅ -alkyl benzene + C ₁₃ H ₂₆ isomers	120	240	C ₁₇ H ₃₄ isomer
105	202	α-methylnaphthalene	120A	240	C ₁₇ H ₃₆ isomer
			121	240	sat. hydrocarbon
			122	240	C ₁₅ H ₃₀ O isomer
			123	240	n-heptadecane
			124	240	C ₁₉ H ₄₀ isomer

Table C-9. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 2, P2/L5).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	26	133	n-nonane
4	52	n-propane (tent.)	27	137	C ₁₀ H ₂₂ isomer
4A	53	butene	27A	140	C ₁₀ H ₂₂ isomer
5	53	n-butane	27B	141	C ₁₀ H ₁₆ isomer
6	55	acetaldehyde	27C	142	C ₈ H ₁₆ O isomer
7	58	isopentane	28	143	benzaldehyde
7A	58	dimethyl ether	28A	143	n-propylbenzene
8	59	acetone	28B	144	ethyltoluene isomer
8A	61	dichloroethylene isomer	29	146	C ₁₁ H ₂₄ isomer
9	62	dichloromethane	29A	147	phenol
10A	65	C ₄ H ₈ O isomer	29B	148	C ₃ -alkyl benzene isomer
10B	68	C ₆ H ₁₂ isomer (tent.)	30	149	C ₁₁ H ₂₄ isomer
11	68	2-methylpentane	31	150	n-octanal
12	70	3-methylpentane	31A	150	C ₁₀ H ₂₀ isomer
13	72	hexafluorobenzene (e8)	31B	151	1,2,4-trimethylbenzene
14	73	n-hexane	32	152	n-decane
14A	73	diisopropyl ether	32A	155	1,2,3-trimethylbenzene + C ₁₁ H ₂₄ isomer
15	74	chloroform	33	157	C ₁₁ H ₂₄ isomer
15A	75	ethyl acetate (tent.)	33A	159	unsat. hydrocarbon
16	77	perfluorotoluene (e8)	34	160	sat. hydrocarbon
16A	78	methylcyclopentane	34A	161	C ₄ -alkyl benzene isomer
17	83	benzene	35	162	acetophenone
17A	84	carbon tetrachloride	35A	163	cresol isomer
17B	94	cyclohexane	35B	164	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers
17C	95	2-methylhexane	35C	165	C ₄ -alkyl benzene isomer
18	87	C ₇ H ₁₆ isomer	35D	166	C ₁₁ H ₂₂ isomer
18A	89	C ₇ H ₁₄ isomer (tent.)	35E	166	C ₄ -alkyl benzene isomer
19	90	acetic acid	36	167	n-nonanal
20	92	n-heptane	36A	168	C ₁₁ H ₂₂ isomer
20A	93	C ₇ H ₁₄ + C ₅ H ₁₀ O isomers (tent.)	37	169	n-undecane
20B	97	methylcyclohexane	37A	172	C ₄ -alkyl benzene isomer
20C	99	C ₇ H ₁₀ isomer (tent.)	37B	174	C ₁₂ H ₂₄ isomer
20D	102	C ₈ H ₁₆ isomer	38	175	dimethylphenol isomer
20E	102	C ₈ H ₁₈ isomer	38A	176	C ₁₂ H ₂₄ isomer
21	104	toluene	38B	177	C ₁₂ H ₂₆ isomer
21A	105	C ₈ H ₁₈ isomer	39	178	C ₂ -alkyl phenol isomer
21B	107	C ₈ H ₁₈ isomer	39A	180	C ₄ -alkyl benzene + C ₁₂ H ₂₄ isomers
22	110	n-hexanal	39B	182	C ₃ -alkyl phenol isomer
23	113	n-octane	40	184	n-decanal + naphthalene
23A	115	tetrachloroethylene (tent.)	40A	185	C ₁₂ H ₂₄ isomer
23B	124	ethylbenzene	41	186	n-dodecane
24	126	xylene isomer	41A	187	C ₃ -alkyl phenol isomer
24A	129	C ₉ H ₂₀ isomer	41B	188	C ₁₂ H ₂₄ isomer
24B	130	styrene			
24C	131	n-heptanal			
25	131	o-xylene + C ₉ H ₂₀ isomer			

(continued)

Table C-9. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
41C	193	C ₁₂ H ₂₄ isomer	44	207	alkyl butyrate
41D	197	C ₁₁ H ₂₀ O isomer (tent.)	44A	208	biphenyl (tent.)
41E	198	C ₁₃ H ₂₆ isomer	44B	209	C ₁₄ H ₂₈ isomer
42	199	<u>n</u> -undecanal	45	210	<u>n</u> -tetradecane
43	200	<u>n</u> -tridecane	47	222	sat. hydrocarbon
43A	201	β -methylnaphthalene	47A	223	C ₁₅ H ₃₀ isomer
43B	205	C ₁₄ H ₃₀ isomer			

Table C-10. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 3, P1/L8).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	7	60	n-pentane
3	51	acetaldehyde	7A	60	dichloroethylene isomer
3A	52	C ₄ H ₈ isomer	7B	61	methylene chloride
4	53	isobutane	7C	61	C ₅ H ₁₀ isomer
4A	54	C ₄ H ₈	9	67	2-methylpentane
4B	55	C ₄ H ₈	10	69	3-methylpentane
5	56	n-butane	11	70	hexafluorobenzene (e3)
5A	56	C ₅ H ₁₀	12	71	n-hexane
6	57	isopentane	13	75	perfluorotoluene (e3)
6A	59	acetone	14	76	methylcyclopentane

Table C-11. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 3, P1/L8).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	27A	118	C ₈ H ₁₆ isomer
3	53	propane	28	119	2-methoxy-2h-dihydro-pyran
3A	55	C ₄ H ₁₀ isomer	28A	122	C ₉ H ₂₀ isomer
3B	56	acetaldehyde	29	123	C ₈ H ₁₆ isomer
3C	56	butane	29A	124	chlorobenzene + ethylcyclo- hexane
4	58	isopentane	29B	125	C ₉ H ₁₈ isomer
5	59	methyl acetate (tent)	30	127	ethylbenzene
5A	60	dimethyl ether	31	129	xylene isomer
5B	60	acetone	31A	129	C ₉ H ₂₀ isomer
6	62	n-pentane	32	130	C ₉ H ₂₀ isomer
6A	63	C ₄ H ₁₀ O isomer (tent)	32A	130	heptanone isomer
7	63	methylene chloride	33	132	styrene
7A	69	C ₆ H ₁₂ isomer	34	133	o-xylene
7B	69	C ₅ H ₁₀ isomer	34A	134	C ₉ H ₁₈ isomer
10	70	2-methylpentane	35	135	n-nonane
10A	71	C ₆ H ₁₂ isomer	36	138	C ₉ H ₁₈ isomer
11	73	3-methylpentane	37	139	isopropylbenzene + C ₁₀ H ₂₂ isomer
11A	73	butanal (tent)	37A	140	C ₁₀ H ₂₂ isomer
11B	73	C ₆ H ₁₂ isomer	38	142	C ₁₀ H ₂₂ + C ₃ -alkyl cyclohexane isomers
12	75	hexafluorobenzene (e3)	38A	143	C ₁₀ H ₁₆ isomer
12A	75	n-hexane	39	143	benzaldehyde
13	76	isopropyl ether	40	144	n-propylbenzene
13A	76	chloroform	40A	145	ethyltoluene isomer
13B	78	methyl ethyl ketone (tent)	41	146	C ₉ H ₁₈ O ketone isomer
14	80	perfluorotoluene (e3)	41A	147	phenol
14A	81	C ₆ H ₁₂ isomer (tent)	41B	147	cyanobenzene + 1,3,5-trimethyl- benzene
15	83	1,1,1-trichloroethane	42	147	C ₁₀ H ₂₂ isomer
16	86	benzene	42A	148	C ₁₀ H ₂₀ isomer
16A	87	carbon tetrachloride	42B	148	C ₁₀ H ₂₂ isomer
16B	87	cyclohexane	42C	149	o-ethyltoluene
17	88	2-methylhexane	43	149	C ₉ H ₁₈ O ketone isomer
17A	89	2,3-dimethylpentane	43A	150	C ₁₀ H ₂₂ isomer
18	90	3-methylhexane	43B	151	benzofuran + C ₁₀ H ₂₀ isomer
19	92	C ₇ H ₁₄ isomer	44	152	1,2,4-trimethylbenzene
19A	93	C ₅ H ₁₀ O isomer	45	153	n-decane
20	95	n-heptane	46	154	dichlorobenzene isomer
20A	97	C ₆ H ₁₂ O isomer (tent)	46A	155	C ₁₀ H ₂₀ isomer
20B	100	methylcyclohexane	46B	155	C ₄ -alkyl benzene isomer
21	101	4-methyl-2-pentanone	46C	156	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers
22	104	C ₆ H ₁₀ O ketone isomers (tent)	-	-	
22A	106	2-hexanol	46D	157	C ₁₀ H ₂₀ isomer
23	108	toluene	47	157	1,2,3-trimethylbenzene
24	110	C ₈ H ₁₈ isomer			
25	113	4-methyl-3-pentan-2-one			
26	115	n-octane			
27	117	tetrachloroethylene			

(continued)

Table C-11. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
47A	157	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers	55F	178	C ₄ H ₇ -benzene isomer
48	159	o-dichlorobenzene	55G	178	unsat. hydrocarbon
48A	159	C ₄ -alkyl cyclohexane isomer + indan	56	180	C ₁₂ H ₂₆ isomer
48B	160	C ₁₁ H ₂₄ isomers	56A	180	C ₅ -alkyl benzene isomer
48C	161	indene + C ₁₁ H ₂₂ isomers	57	181	1,2,3,4-tetrahydronaphthalene
48D	161	C ₃ -alkyl pyridine isomer (tent)	57A	183	C ₅ -alkyl benzene isomer
48E	161	C ₄ -alkyl benzene isomer	58	185	naphthalene
48F	162	C ₄ -alkyl benzene isomer	58A	186	2,3-benzothiophene (tent)
49	162	acetophenone	59	187	n-dodecane
49A	163	C ₄ -alkyl benzene isomer	60	188	2,6,8-trimethylnonanone-4
50	165	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers	60A	192	methylidihydronaphthalene isomer (tent.)
51	166	C ₁₁ H ₂₄ isomer	60B	196	C ₁₂ H ₂₄ O isomer (tent)
51A	166	C ₄ -alkyl benzene isomer	60C	198	C ₁₃ H ₂₈ isomer
51B	167	C ₄ H ₇ -benzene isomer	60D	200	unsat. hydrocarbon
52	168	C ₄ -alkyl benzene isomer	61	202	n-tridecane
52A	168	C ₁₁ H ₂₂ isomer	61A	203	β-methylnaphthalene
53	169	n-nonanal	61B	205	α-methylnaphthalene
53A	169	C ₄ H ₇ -benzene isomer	61C	209	C ₁₅ H ₃₂ isomer (tent)
53B	170	C ₁₁ H ₂₂ isomer	62	213	α-tetralone
54	171	n-undecane	63	214	biphenyl
54A	172	C ₄ -alkyl benzene isomer	64	216	diphenyl ether + n-tetradecane
55	173	3,5,5-trimethyl-2-cyclohexen- one	64A	217	C ₁₄ H ₂₈ isomer
55A	174	C ₄ alkyl benzene isomer	64B	218	C ₂ -alkyl naphthalene isomer
55B	175	2-pyrone (tent)	64C	220	C ₂ -alkyl naphthalene isomer
55C	175	C ₁₁ H ₂₀ isomer	64D	228	C ₁₅ H ₃₀ isomer
55D	175	C ₁₁ H ₂₂ isomer	65	229	n-pentadecane
55E	176	C ₅ -alkyl benzene isomer	65A	231	C ₁₄ H ₁₂ isomer
			68	240	benzophenone
			68A	240	C ₁₇ H ₃₆ isomer

Table C-12. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 3, P2/L1).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	37	105	C ₈ H ₁₈ isomer
3	51	propane (tent)	38	106	toluene
4	52	C ₄ H ₁₀ isomer (tent)	39	108	C ₈ H ₁₈ isomer
5	53	acetaldehyde	40	109	C ₈ H ₁₈ isomer
6	56	n-butane	40A	111	C ₈ H ₁₆ isomer
7	58	isopentane	41	112	C ₉ H ₂₀ isomer
9	60	acetone	41A	113	C ₈ H ₁₆ isomer
9A	61	diethyl ether	42	115	n-octane
10	61	n-pentane	43	116	tetrachloroethylene
10A	61	Background peak	43A	117	C ₈ H ₁₆ isomer
11	62	methylene chloride	43B	119	C ₉ H ₂₀ isomer
13	65	C ₆ H ₁₄ isomer (tent)	43C	120	C ₉ H ₂₀ isomer
14A	68	C ₅ H ₁₀ isomer	43D	121	C ₉ H ₂₀ isomer
15	69	2-methylpentane	43E	122	C ₈ H ₁₆ isomer
16	71	3-methylpentane	44	123	ethylcyclohexane + C ₉ H ₂₀ isomers
16A	72	C ₆ H ₁₂ isomer	44A	124	C ₉ H ₁₈ isomer
17	73	hexafluorobenzene (e#)	44B	125	C ₉ H ₁₈ isomer
18	74	n-hexane	45	127	ethylbenzene
19	75	chloroform	45A	127	C ₉ H ₁₈ isomer
20	76	ethyl acetate	46	128	xylene isomer
20A	77	C ₆ H ₁₂ isomer	46A	129	C ₉ H ₂₀ isomer
21	78	perfluorotoluene (e#)	47	130	C ₉ H ₂₀ isomer
22	79	methylcyclopentane	47A	132	C ₉ H ₂₀ isomer
23	80	unsat. hydrocarbon (tent)	48	132	styrene
24	81	1,1,1-trichloroethane	49	133	o-xylene
24A	82	C ₇ H ₁₄ isomer	49A	134	C ₁₀ H ₂₂ isomer
24B	83	C ₆ H ₁₀ isomer	49B	134	C ₉ H ₁₈ isomer
25	84	benzene	50	136	n-nonane
26	85	carbon tetrachloride	50A	138	C ₉ H ₁₈ isomer
26A	86	cyclohexane	51	139	C ₁₀ H ₂₂ isomer + isopropyl- benzene
27	86	2-methylhexane	51A	140	C ₁₀ H ₂₀ isomer
27A	87	2,3-dimethylpentane	52	141	C ₁₀ H ₂₂ isomer
28	87	acetic acid	53	143	C ₁₀ H ₂₂ isomer
29	88	3-methylhexane	53A	143	C ₁₀ H ₂₀ isomer
30	90	C ₇ H ₁₄ isomer	54	144	C ₁₀ H ₁₆ isomer
30A	91	C ₇ H ₁₄ isomer	55	144	benzaldehyde
31	91	C ₈ H ₁₈ isomer	56	145	n-propylbenzene
31A	92	C ₇ H ₁₄ isomer	57	146	ethyltoluene isomer
32	93	n-heptane	57A	147	C ₁₀ H ₂₂ isomer
33	94	C ₇ H ₁₄ isomer	57B	148	phenol
34	99	methylcyclohexane	57C	148	1,3,5-trimethylbenzene
34A	100	C ₈ H ₁₆ isomer	58	148	C ₁₁ H ₂₄ isomer
35	101	C ₈ H ₁₈ isomer	58A	150	C ₁₀ H ₂₂ isomer
35A	102	C ₆ H ₁₂ O isomer	58B	150	o-ethyltoluene
36	103	C ₈ H ₁₆ isomer			
36A	104	C ₈ H ₁₆ isomer			

continued

Table C-12. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
58C	151	C ₁₀ H ₂₂ isomer	70D	179	C ₅ -alkyl benzene isomer
58D	152	C ₁₀ H ₁₆ isomer	70E	180	C ₅ -alkyl cyclohexane isomer
58E	152	C ₃ H ₅ -benzene + C ₁₀ H ₂₀ isomers	70F	180	C ₁₂ H ₂₄ + C ₅ -alkyl benzene isomers
59	153	1,2,4-trimethylbenzene	70G	181	C ₄ H ₇ -benzene isomer
59A	154	C ₁₀ H ₂₀ isomer	71	182	C ₁₂ H ₂₆ + C ₅ -alkyl benzene isomers
60	155	n-decane	71A	182	C ₁₂ H ₂₄ isomer
61	156	dichlorobenzene isomer	71B	183	C ₄ -alkyl benzene isomer
61A	156	C ₁₀ H ₂₀ isomer	71C	183	C ₅ -alkyl benzene isomer
61B	157	C ₄ -alkyl benzene isomer	71D	184	C ₁₂ H ₂₆ isomer
61C	158	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers	71E	184	C ₅ -alkyl benzene isomer
62	158	1,2,3-trimethylbenzene	71F	185	C ₁₀ H ₂₀ O isomer
62A	159	C ₁₁ H ₂₄ isomer	71G	186	naphthalene
63	160	C ₁₂ H ₂₆ isomer	72	187	n-decanal
63A	161	indan	72A	187	C ₁₂ H ₂₄ isomer
63B	162	C ₄ -alkyl cyclohexane isomer	72B	188	C ₅ -alkyl benzene isomer
63C	162	C ₁₁ H ₂₂ isomer	73	189	n-dodecane
63D	163	C ₄ -alkyl benzene isomer	73A	190	C ₅ -alkyl benzene isomer
64	163	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers	73B	190	C ₁₂ H ₂₄ isomer
65	164	acetophenone	73C	196	C ₁₃ H ₂₈ isomer
65A	164	C ₄ -alkyl benzene isomer	73D	200	C ₁₃ H ₂₈ isomer
65B	165	C ₁₁ H ₂₄ isomer	73E	202	C ₁₂ H ₂₄ isomer
65C	165	C ₁₁ H ₂₂ isomer	74	204	n-tridecane
66	166	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers	74A	204	β-methylnaphthalene
66A	168	C ₁₁ H ₂₄ isomer	74B	205	C ₁₃ H ₂₆ isomer
66B	168	C ₄ -alkyl benzene isomer	74C	206	α-methylnaphthalene
66C	169	C ₁₂ H ₂₄ isomer	75	211	C ₅ -alkyl cyclohexane isomer
66D	169	C ₄ H ₇ -benzene isomer	75A	216	C ₁₄ H ₂₈ isomer
67	169	C ₄ -alkyl benzene isomer	76	218	n-tetradecane
67A	170	C ₁₂ H ₂₆ isomer	76A	220	dimethylnaphthalene isomer
68	170	n-nonanal	76B	222	dimethylnaphthalene isomer
68A	171	C ₁₁ H ₂₂ isomer	76C	224	C ₁₅ H ₃₀ isomer
69	172	n-undecane	76D	230	C ₁₅ H ₃₀ isomer
69A	173	C ₅ -alkyl benzene isomer	77	231	n-pentadecane
69B	173	C ₄ -alkyl benzene isomer	78	235	unknown
69C	174	C ₁₁ H ₂₂ isomer	79A	240	C ₁₆ H ₃₂ isomer
70	176	C ₄ -alkyl benzene isomer	80A	240	n-hexadecane
70A	177	C ₁₂ H ₂₆ isomer	80B	240	benzophenone
70B	178	C ₂ -alkyl phenol isomer			
70C	178	C ₅ -alkyl benzene isomer			

Table C-13. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 3, P2/L2).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	25	111	C ₈ H ₁₈ isomer
3A	52	propane (tent)	25A	112	C ₆ H ₁₂ O isomer
3B	52	C ₄ H ₈ isomer	25B	112	C ₈ H ₁₆ isomer
4	53	C ₄ H ₁₀ isomer	26	113	n-hexanal + C ₉ H ₂₀ isomer
4A	54	acetaldehyde	26A	114	C ₈ H ₁₆ isomer
4B	59	isopentane	27	116	n-octane
4C	61	C ₅ H ₁₀ isomer	28	117	tetrachloroethylene
4D	61	furan (tent)	28A	118	C ₈ H ₁₆ isomer
5	62	acetone + n-pentane	28B	119	C ₉ H ₂₀ isomer (tent)
5A	63	diethyl ether (tent)	29	119	C ₉ H ₂₀ isomer
5B	64	dichloroethylene isomer (traces)	29A	121	C ₉ H ₂₀ isomer
6	64	methylene chloride	29B	121	C ₈ H ₁₆ isomer
7A	71	C ₅ H ₁₀ isomer	30	122	C ₉ H ₂₀ isomer
8	71	2-methylpentane	30A	123	C ₉ H ₁₈ isomer
8A	73	C ₅ H ₁₀ O isomer	31	124	C ₉ H ₂₀ isomer + ethylcyclo- hexane
9	74	3-methylpentane	31A	125	C ₉ H ₁₈ isomer
9A	74	butanal	31B	126	C ₇ H ₁₄ O isomer (tent)
9B	75	C ₆ H ₁₂ isomer	32	127	ethylbenzene isomer
10	76	hexafluorobenzene (e8)	32A	128	C ₉ H ₁₈ isomer
11	77	n-hexane	33	129	xylene isomer
12	77	chloroform	33A	129	C ₉ H ₂₀ isomer
12A	80	C ₆ H ₁₂ isomer	34	130	C ₉ H ₂₀ isomer
13	81	perfluorotoluene (e8)	34A	131	C ₇ H ₁₄ O isomer
14	82	methylcyclopentane	35	132	C ₁₀ H ₂₂ isomer
14A	84	1,1,1-trichloroethane	35A	132	styrene
14B	86	C ₆ H ₁₀ isomer (tent)	35B	133	C ₉ H ₁₈ isomer
15	87	benzene	36	133	o-xylene
15A	88	carbon tetrachloride (traces)	36A	134	C ₉ H ₁₈ isomer
15B	88	cyclohexane	37	136	n-nonane
16	89	2-methylhexane	38	138	C ₉ H ₁₈ isomer
16A	90	2,3-dimethylpentane (tent)	39	139	C ₁₀ H ₂₂ isomer + isopropyl- benzene
17	91	3-methylhexane + acetic acid	39A	140	C ₁₀ H ₂₀ isomer
18	93	C ₇ H ₁₄ isomer	40	141	C ₁₀ H ₂₂ isomer
18A	94	trichloroethylene	40A	141	C ₉ H ₁₆ isomer (tent)
18B	94	C ₈ H ₁₈ isomer	40B	142	C ₁₀ H ₂₂ isomer
19	96	n-heptane	41	142	C ₁₀ H ₂₂ isomer
19A	98	C ₇ H ₁₄ isomer	41A	143	C ₃ -alkyl cyclohexane isomer
20	101	methylcyclohexane	42	144	benzaldehyde
21	103	C ₈ H ₁₈ isomer	42A	145	C ₁₀ H ₂₀ isomer
21A	103	C ₆ H ₁₂ O ketone isomer	43	145	n-propylbenzene
21B	105	C ₈ H ₁₆ isomer	44	146	ethyltoluene isomer
21C	106	C ₈ H ₁₆ isomer	44A	147	C ₁₀ H ₂₂ isomer
22	107	C ₈ H ₁₈ isomer	45	148	1,3,5-trimethylbenzene
23	108	toluene	45A	148	C ₁₁ H ₂₄ isomer
24	109	C ₈ H ₁₈ isomer			

(continued)

Table C-13. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
45B	149	phenol (tent) + C ₁₀ H ₂₀ isomer	66	177	C ₅ -alkyl benzene isomer
46	149	C ₁₀ H ₂₂ isomer	66A	178	C ₄ H ₇ -benzene isomer
47	150	<u>o</u> -ethyltoluene	67	178	C ₅ -alkyl benzene isomer
47A	151	C ₁₀ H ₂₂ isomer	67A	178	C ₄ H ₇ -benzene isomer
47B	151	C ₁₁ H ₂₄ isomer	67B	179	C ₁₂ H ₂₄ isomer
48	152	<u>n</u> -octanal	68	179	C ₅ -alkyl benzene isomer
49	153	1,2,4-trimethylbenzene	69	180	C ₄ H ₇ -benzene isomer
49A	153	C ₁₀ H ₂₀ isomer	70	181	C ₄ -alkyl benzene isomer
50	154	<u>n</u> -decane	70A	181	C ₅ -alkyl benzene isomer
51	155	dichlorobenzene isomer	70B	182	C ₅ -alkyl benzene isomer
51A	155	isobutylbenzene	71	182	1,2,3,4-tetrahydronaphthalene
51B	156	sec-butylbenzene	71A	182	C ₅ -alkyl benzene isomer
52	157	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers	72	183	C ₅ -alkyl benzene isomer
53	158	1,2,3-trimethylbenzene	72A	184	C ₄ -alkyl benzene isomer
53A	158	C ₁₁ H ₂₄ isomer	72B	185	C ₆ -alkyl benzene isomer
54	159	C ₁₁ H ₂₄ isomer	72C	185	C ₅ H ₉ -benzene + C ₅ -alkyl benzene isomers
55	160	C ₃ H ₅ -benzene isomer	73	186	naphthalene
55A	161	C ₁₁ H ₂₄ isomer	73A	186	C ₅ H ₉ -benzene isomer
55B	161	C ₄ -alkyl cyclohexane isomer	73B	186	C ₅ -alkyl benzene isomer
55C	161	C ₁₁ H ₂₂ isomer	74	187	C ₅ -alkyl benzene isomer + <u>n</u> -dodecane
55D	162	C ₄ -alkyl benzene isomer	74A	188	C ₆ -alkyl benzene isomer
56	162	<u>p</u> -propyltoluene	75	189	C ₅ -alkyl benzene isomer
57	163	C ₄ -alkyl benzene isomer + acetophenone (tent.)	75A	190	C ₁₃ H ₂₈ isomer
57A	164	C ₄ -alkyl benzene isomer	76	191	C ₆ -alkyl benzene isomer
57B	164	C ₁₁ H ₂₄ isomer	76A	192	C ₅ -alkyl benzene isomer
58	166	<u>o</u> -propyltoluene	76B	193	C ₅ -alkyl benzene isomer
58A	167	C ₁₁ H ₂₄ isomer	77	194	C ₁₃ H ₂₆ isomer
59	167	C ₄ -alkyl benzene isomer	77A	195	C ₆ -alkyl benzene isomer
59A	168	C ₁₁ H ₂₄ isomer	77B	195	C ₅ -alkyl benzene isomer
60	169	C ₄ -alkyl benzene isomer	77C	195	C ₁₃ H ₂₈ isomer
60A	169	<u>n</u> -nonanal + C ₄ H ₇ -benzene isomer	77D	196	C ₅ H ₉ -benzene isomer
61	170	C ₄ -alkyl benzene isomer	77E	196	C ₆ -alkyl benzene isomer
61A	170	C ₁₁ H ₂₂ isomer	77F	196	C ₅ -alkyl benzene isomer
62	171	<u>n</u> -undecane + C ₅ -alkyl benzene isomer	77G	197	C ₁₃ H ₂₈ isomer
63	172	C ₄ -alkyl benzene isomer	77H	197	C ₅ -alkyl benzene isomer
63A	173	C ₁₁ H ₂₂ isomer	78	199	C ₁₄ H ₃₀ isomer
63B	173	C ₅ -alkyl benzene isomer	78A	200	C ₁₃ H ₂₆ isomer
63C	173	C ₁₂ H ₂₄ isomer	78B	200	C ₅ -alkyl benzene isomer
63D	174	C ₁₂ H ₂₆ isomer	78C	201	C ₁₃ H ₂₆ isomer
64	174	tetramethylbenzene isomer	79	202	<u>n</u> -tridecane
65	175	C ₄ -alkyl benzene isomer	79A	203	β -methylnaphthalene
65A	176	C ₁₂ H ₂₆ isomer	80	204	C ₅ -alkyl benzene isomer
			80A	205	C ₆ -alkyl benzene isomer
			81	205	α -methylnaphthalene

(continued)

Table C-13. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
81A	209	C ₅ H ₉ -benzene + C ₆ -alkyl benzene isomers	84D	223	C ₁₅ H ₃₀ isomer
82	210	C ₆ -alkyl benzene isomer	84E	225	C ₁₅ H ₃₂ isomers
83	213	1,2,3,4-tetrahydronaphthalen- 1-one	84F	227	C ₁₃ H ₂₆ O isomer
83A	214	biphenyl	84G	228	C ₁₅ H ₃₀ isomer
83B	214	C ₁₄ H ₃₀ isomer	85	229	n-pentadecane
83C	215	C ₁₄ H ₂₈ isomer	86	233	unknown
84	216	n-tetradecane	88A	240	n-hexadecane
84A	218	C ₁₀ H ₁₀ O isomer (tent)	88B	240	benzophenone
84B	219	dimethylnaphthalene isomer	88C	240	C ₁₇ H ₃₆ isomer
84C	220	dimethylnaphthalene isomer	88D	240	alkyl ketone
			88E	240	n-heptadecane

Table C-14. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN THE KANAWHA VALLEY, WV (TRIP 3, P2/L9).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	47	CO ₂	11	64	CS ₂
3	51	propane	12	69	2-methylpentane
4	53	isobutane	13	71	3-methylpentane
4A	54	C ₄ H ₁₀ isomer	13A	72	C ₅ H ₁₂ isomer
5	56	n-butane	14	73	hexafluorobenzene (e ₂)
6	58	isopentane	15	74	n-hexane
7	59	acetone	15A	75	chloroform
8	60	n-pentane	16	76	C ₇ H ₁₆ isomer (tent.)
8A	61	diethyl ether	17	78	perfluorotoluene (a ₂)
8B	62	vinylidene chloride	18	79	methylcyclopentane
9	62	methylene chloride			

APPENDIX D

SEMIVOLATILE COMPOUNDS IDENTIFIED IN AIR PARTICULATE COLLECTED
IN KANAWHA VALLEY, WV

Table D-1. COMPOUNDS IDENTIFIED IN POLAR NEUTRAL FRACTION OF <1.7 μ
AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV
(Trip 3, P1/L1)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	124	naphthalene	18	259	a phthalate
2	135	benzothiazole (tent.)	19	263	a phthalate
3	161	Si compound (bkg.)	20	265	C ₁₈ H ₁₀ isomer ⁴ (tent.)
4	167	C ₄ alkyl benzene	21	265	C ₁₈ H ₁₄ isomer ⁵
5	168	naphthol + unknown	22	265	C ₁₈ H ₁₀ isomer ⁴ (tent.)
6	182	unknown	23	265	C ₁₈ H ₁₂ isomer ⁶
7	196	p-nonyl phenol	24	265	benzanthrone
8	202	C ₁₄ H ₁₀ isomer	25	265	a phthalate (bkg.)
9	212	a phthalate (bkg.)	26	265	methylbenzanthracene isomer or methylbenzophenanthrene isomer ⁷
10	213	C ₁₃ H ₉ N isomer ¹ (tent.)	27		triphenylphosphine sulfide (bkg.)
11	216	C ₁₃ H ₈ O isomer ² (tent.)	28	265	unknown
12	217	C ₂ alkyl fluorene (tent.)	29	265	C ₂₀ H ₁₂ isomer ⁸
13	221	methyl hexadecanoate	30	265	C ₂₀ H ₁₂ isomer ⁸ (tent.)
14	222	a phthalate (bkg.)	31	265	C ₂₀ H ₁₂ isomer ⁸
15	234	C ₁₆ H ₁₀ isomer ³	32	265	binaphthyl isomer + unknown
16	239	C ₁₆ H ₁₀ isomer ³	33	265	unknown
17	243	methyl octadecanoate + unknown(s)			

1. C₁₃H₉H isomers include benzoquinoline isomers and acridine.
2. C₁₃H₈O isomers include fluorenones and perinaphthindenones and benzoindenones.
3. C₁₆H₁₀ isomers include pyrene and fluoranthene.
4. C₁₈H₁₀ isomers include 1,10-benzfluoranthene, 3,4-cyclopentapyrene and 1,10-benzoaceanthrylene.
5. C₁₈H₁₄ isomers include terphenyl isomers.
6. C₁₈H₁₂ isomers include benzanthracene isomers (naphthacene et al.) and benzophenanthrene isomers (triphenylene, chrysene et al.)
7. This compound is not a methylchrysene or a methyltriphenylene.
8. C₂₀H₁₂ isomers include perylene, benzpyrene isomers, and benzfluoranthene isomers.

Table D-2. COMPOUNDS IDENTIFIED IN PNA FRACTION OF <1.7 μ
AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV
(Trip 3, P1/L1)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	111	unknown + dichloromethane (solvent)	41	243	trimethylphenanthrene isomer
2	116	Si compound (bkg.)	42	244	trimethylphenanthrene isomer.
3	122	unknown	43	246	trimethylphenanthrene isomer
4	123	naphthalene	44	247	benzofluorene isomer
5	124	Si compound (bkg.)	45	249	C ₁₇ H ₁₂ isomer ⁴
6	125	unknown	46	251	methylpyrene isomer (tent.)
7	132	unknown	47	252	methylpyrene isomer (tent.)
8	143	unknown	48	255	methylpyrene isomer
9	144	methylnaphthalene isomer (tent.)	49	261	C ₄ alkyl C ₁₄ H ₁₀ isomer (tent.)
10	151	C ₁₂ H ₁₀ isomer	50	264	a phthalate
11	155	unknown	51	265	terphenyl isomer (tent.)
12	156	dimethylnaphthalene isomer + unknown	52	265	terphenyl isomer (tent.)
13	159	biphenylene (tent.)	53	265	C ₁₈ H ₁₀ isomer ⁵
14	160	unknown	54	265	terphenyl isomer
15	162	di-t-butylbenzoquinone (bkg.?)	55	265	C ₁₈ H ₁₀ isomer ⁵
16	168	dibenzofuran (tent.)	56	265	C ₁₈ H ₁₂ isomer ⁶
17	169.5	unknown	57	265	a phthalate (bkg.)
18	173	trimethylnaphthalene isomer (tent.) + a phthalate (bkg.)	58	265	unknown
19	175	C ₃ alkyl naphthalene (tent.)	59	265	unknown
20	177	fluorene	60	265	C ₁₉ H ₁₄ isomer ⁷ (tent.)
21	181	2,2,4-trimethylpenta-1,3-diol di-isobutyrate (bkg.)	61	265	phthalate(s) (bkg.)
22	184	hydroxyfluorene (tent.)	62	265	phthalate(s) (bkg.)
23	191	C ₄ alkyl naphthalene (tent.)	63	265	C ₁₉ H ₁₄ isomer ⁷ (tent.)
24	193	methylfluorene isomer (tent.)	64	265	methyl C ₁₈ H ₁₀ isomer ⁵ (tent.) + C ₂ alkyl terphenyl (tent.)
25	195	unknown	65	265	C ₂ alkyl C ₁₈ H ₁₂ isomer ⁶
26	201	C ₁₄ H ₁₀ isomer ²	66	265	C ₂ alkyl C ₁₈ H ₁₂ isomer ⁶
27	208	dimethylfluorene + unknown	67	265	C ₂ alkyl C ₁₈ H ₁₂ isomer ⁶
28	211	methyldibenzothiophene isomer (tent.)	68	265	C ₂₂ H ₁₂ isomer ⁸ (tent.)
29	212	a phthalate (bkg.)	69	265	C ₂₀ H ₁₂ isomer ⁹
30	216	methyl C ₁₄ H ₁₀ isomer ²	70	265	C ₂₂ H ₁₂ isomer ⁸ (tent.)
31	217	4,5-methylenephenanthrene	71	265	C ₂₁ H ₂₀ isomer ¹⁰ (tent.)
32	219	methyl C ₁₄ H ₁₀ isomer ²	72	265	C ₂₀ H ₁₂ isomer ⁹ (tent.)
33	211	unknown(s)	73	265	C ₂ alkyl C ₁₈ H ₁₂ isomer ⁶ (tent.)
34	222	a phthalate (bkg.)	74	265	C ₂₂ H ₁₂ isomer(s) ⁸ (tent.)
35	229	dimethylphenanthrene isomer	75	265	C ₂₁ H ₁₆ isomer ¹¹ (tent.)
36	230	diphenyloxazole isomer(s) (tent.)	76	265	C ₂₁ H ₁₇ isomer ¹¹ (tent.)
37	231	dimethylphenanthrene isomer	77	265	C ₂₂ H ₁₂ isomer ⁸ (tent.)
38	233	C ₁₆ H ₁₀ isomer ³	78	265	C ₂₀ H ₁₄ isomer ¹² (tent.)
39	236	C ₁₆ H ₁₀ isomer ³	79	265	C ₂₀ H ₁₂ isomer ⁹ (tent.)
40	239	C ₁₆ H ₁₀ isomer ³	80	265	C ₂₂ H ₁₂ isomer ⁸ (tent.)
			81	265	C ₂₁ H ₁₆ isomer ¹¹ (tent.)
			82	265	C ₂₁ H ₁₈ isomer ¹³ (tent.)
			83	265	C ₂₃ H ₁₄ isomer ¹⁴ (tent.)
			84	265	C ₂₀ H ₁₂ isomer ⁹ (tent.)
			85	265	C ₂₁ H ₁₆ isomer ¹¹ (tent.)

(continued)

Table D-2. (cont'd)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
86	265	C ₂₁ H ₁₄ isomer(s) ¹⁵ (tent.)	92	265	C ₂₁ H ₁₄ isomer ¹⁵ (tent.)
87	265	C ₂₁ H ₁₈ isomer ¹³ (tent.)	93	265	C ₂₂ H ₁₈ isomer ¹⁷ (tent.)
88	265	C ₂₁ H ₁₄ isomer ¹⁵ (tent.)	94	265	unknown
89	265	C ₂₄ H ₁₈ isomer ¹⁶ (tent.)	95	265	methyl C ₂₀ H ₁₂ isomer ⁹ (tent.)
90	265	C ₂₁ H ₁₆ isomer ¹¹ (tent.)	96	265	unknown
91	265	C ₄ alkyl C ₁₈ H ₁₂ isomer ⁶ (tent.)			

- C₁₂H₁₀ isomers include biphenyl and acenaphthene.
- C₁₄H₁₀ isomers include diphenylacetylene, phenanthrene and anthracene.
- C₁₆H₁₀ isomers include fluorene, pyrene, benz[a]acenaphthene and benz[e] acenaphthene.
- C₁₇H₁₂ isomers include benzofluorene isomers and methyl C₁₆H₁₀ isomers.
- C₁₈H₁₀ isomers include 1,10-benzfluorene, 3,4-cyclopentapyrene and 1,10-benzoaceanthrylene.
- C₁₈H₁₂ isomers include benzanthracene isomers, benzophenanthrene isomers, triphenylene and chrysene.
- C₁₉H₁₄ isomers include methyl C₁₈H₁₂ isomers.
- C₂₂H₁₂ isomers include 1,12-benzperylene; 2,3-o-phenylenepyrene; anthanthrene and indeno[1,2,3-cd]pyrene.
- C₂₀H₁₂ isomers include perylene; benzfluorene isomers; benzpyrene isomers and benzaceanthrylene isomers.
- C₂₁H₂₀ isomers include C₃ alkyl terphenyl isomers; C₃ alkyl styrylnaphthalene isomers and triphenyl C₃ alkane isomers.
- C₂₁H₁₆ isomers include diphenylindene isomers; methylbenzaceanthrene isomers; methylbenzimidine fluorene isomers and dinaphthylmethane isomers.
- C₂₀H₁₄ isomers include acenaphthanthracene; phenylanthracene isomers; binaphthyl isomers; benzaceanthrene isomers; indenofluorene isomers and 9-benzylidene fluorene.
- C₂₁H₁₈ isomers include dihydromethyl C₂₀H₁₄ isomers, tetrahydrocyclohepta-C₁₆H₁₀ isomers and methyl C₂₀H₁₆ isomers.
- C₂₃H₁₄ isomers include methyl C₂₂H₁₂ isomers.
- C₂₁H₁₄ isomers include methyl C₂₀H₁₂ isomers.
- C₂₂H₁₈ isomers include triphenylbenzene isomers (quaterphenyls)
- C₂₂H₁₈ isomers include dihydromethylcycloheptapyrene isomers; C₂₂ alkyl C₂₀H₁₄ isomers and methyl C₂₁H₁₆ isomers.

Table D-3. COMPOUNDS IDENTIFIED IN PARAFFIN FRACTION OF $<1.7 \mu$
AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV
(TRIP 3, P1/L1)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	115	undecane (tent.)	16	265	unknown
2	118	dimethylundecane (tent.)	17	265	C ₂₉ H ₅₂ arene
3	123	an alkane	18	265	C ₃₀ H ₅₄ arene
4	124	an alkane	19	265	mixture of alkanes and alkenes
5	125	an alkane	20	265	C ₂₉ H ₅₂ arene
6	129	n-dodecane	21	265	C ₂₉ H ₅₂ arene
7	131	an alkane	22	265	C ₃₀ H ₅₄ arene
8	165	di-t-butyl-o-benzoquinone isomer + di-t-butyl-p-benzoqui- none isomer	23	265	a phthalate (bkg.)
9	176	an alkane	24	265	C ₂₉ H ₆₀ alkane or C ₃₀ H ₄₈ alkene
10	~215-250	alkanes + alkenes	25	265	C ₃₀ H ₅₄ arene
11	265	a phthalate (bkg.)	26	265	C ₂₆ H ₅₄ alkene (tent.)
12	265	C ₂₆ H ₅₄ alkane	27	265	a phthalate (tent.)
13	265	C ₂₇ H ₄₈ alkene	28	265	unknown
14	265	C ₂₇ H ₅₆ alkane	29	265	C ₃₀ H ₆₂ alkane
15	265	C ₂₈ H ₅₀ alkene	30	265	C ₃₀ H ₃₀ arene (tent.)
			31	265	arene(s)

Table D-4. COMPOUNDS IDENTIFIED IN BASE FRACTION OF $<1.7 \mu$
AIR PARTICULATE COLLECTED IN KANAWHA VALLEY, WV
(TRIP 3, P1/L1)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	125	naphthalene (tent.)	10	198	p-nonylphenol
2	143	quinoline (tent.)	11	201	C ₉ alkyl phenol
3	156	nicotine (tent.)	12	203	C ₉ alkyl phenol
4	164	C ₂ alkyl quinoline (tent.)	13	206	C ₁₃ H ₉ N isomer
5	170	di-t-butylphenol	14	210	C ₁₃ H ₉ N isomer
6	183	2,2,4-trimethylpenta-1,3-diol	15	211	caffeine (tent.)
		di-isobutyrate (bkg.)	16	213	a phthalate (bkg.)
7	191	C ₉ alkyl phenol (tent.)	17	225	a phthalate ester (bkg.)
8	195	unknown	18	233	2,5-diphenyl oxazole
9	196	C ₉ alkyl phenol	19*	265	diocetyl adipate (bkg?)

* Unlabelled peaks beyond file position 400 are phthalates (bkg.)

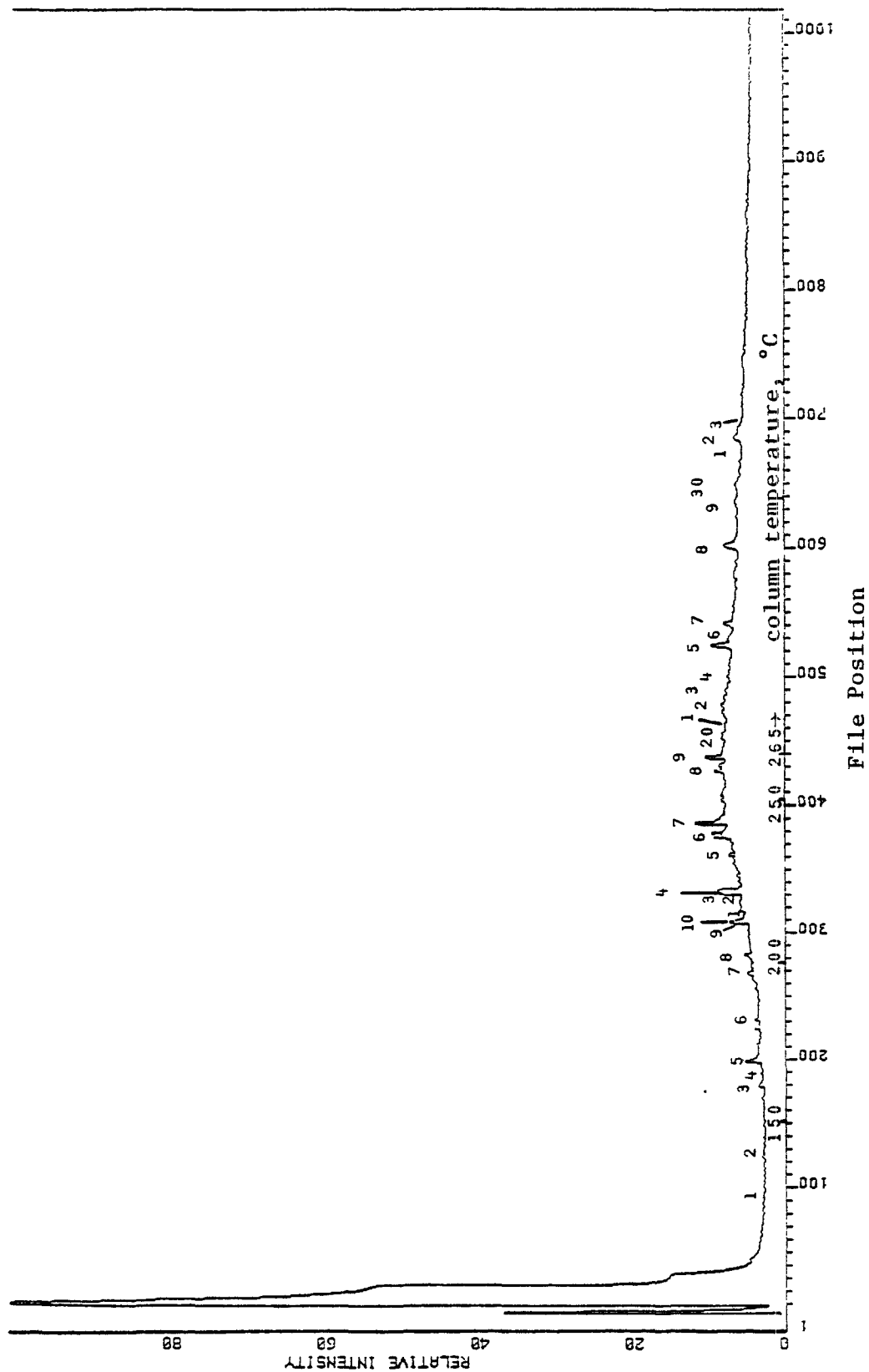


Figure D-1. Total ion current chromatogram of EC/MS/COMP Analysis of Polar Neutral Fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

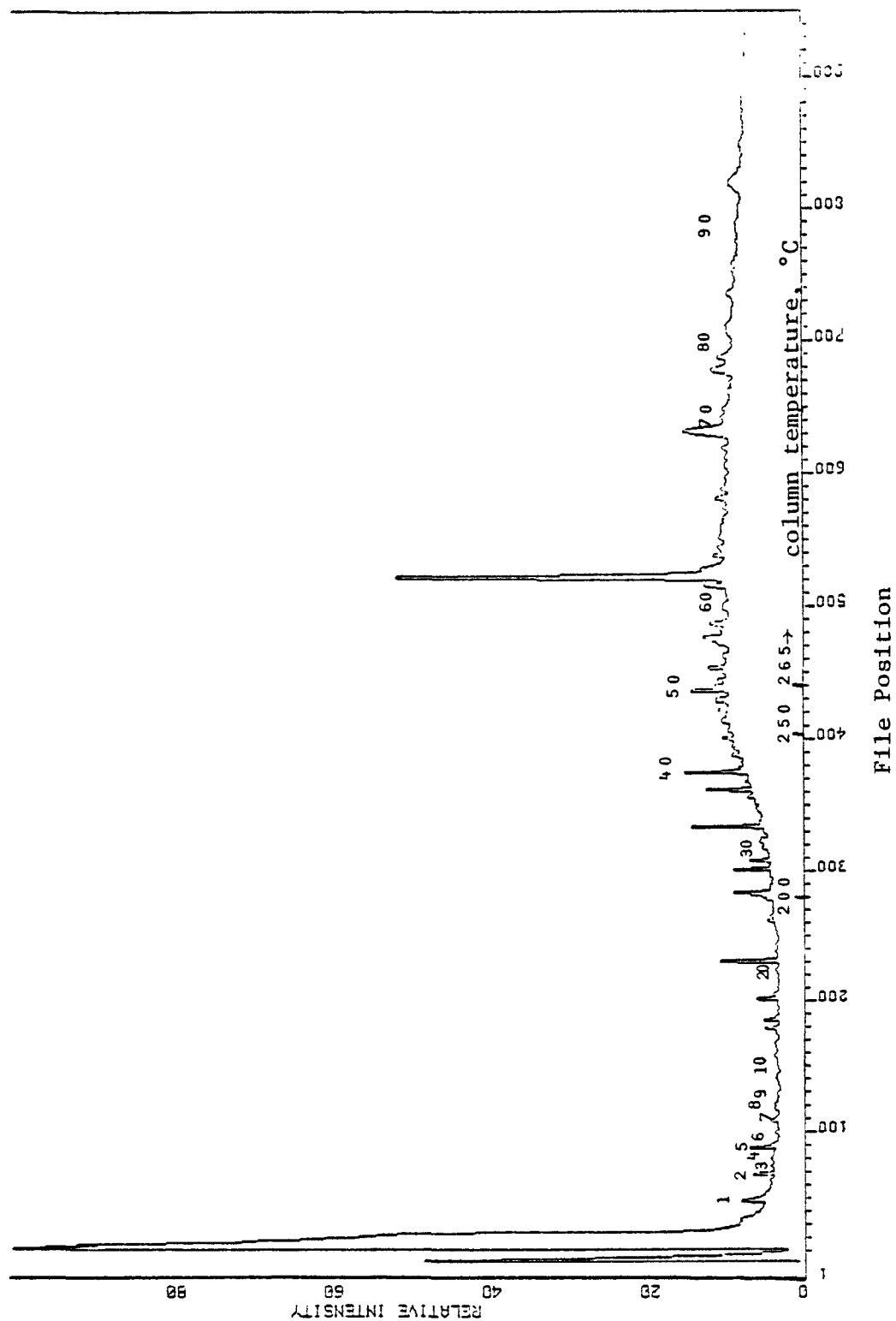


Figure D-2... Total ion current chromatogram of GC/MS/COMP analysis of PNA fraction
of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

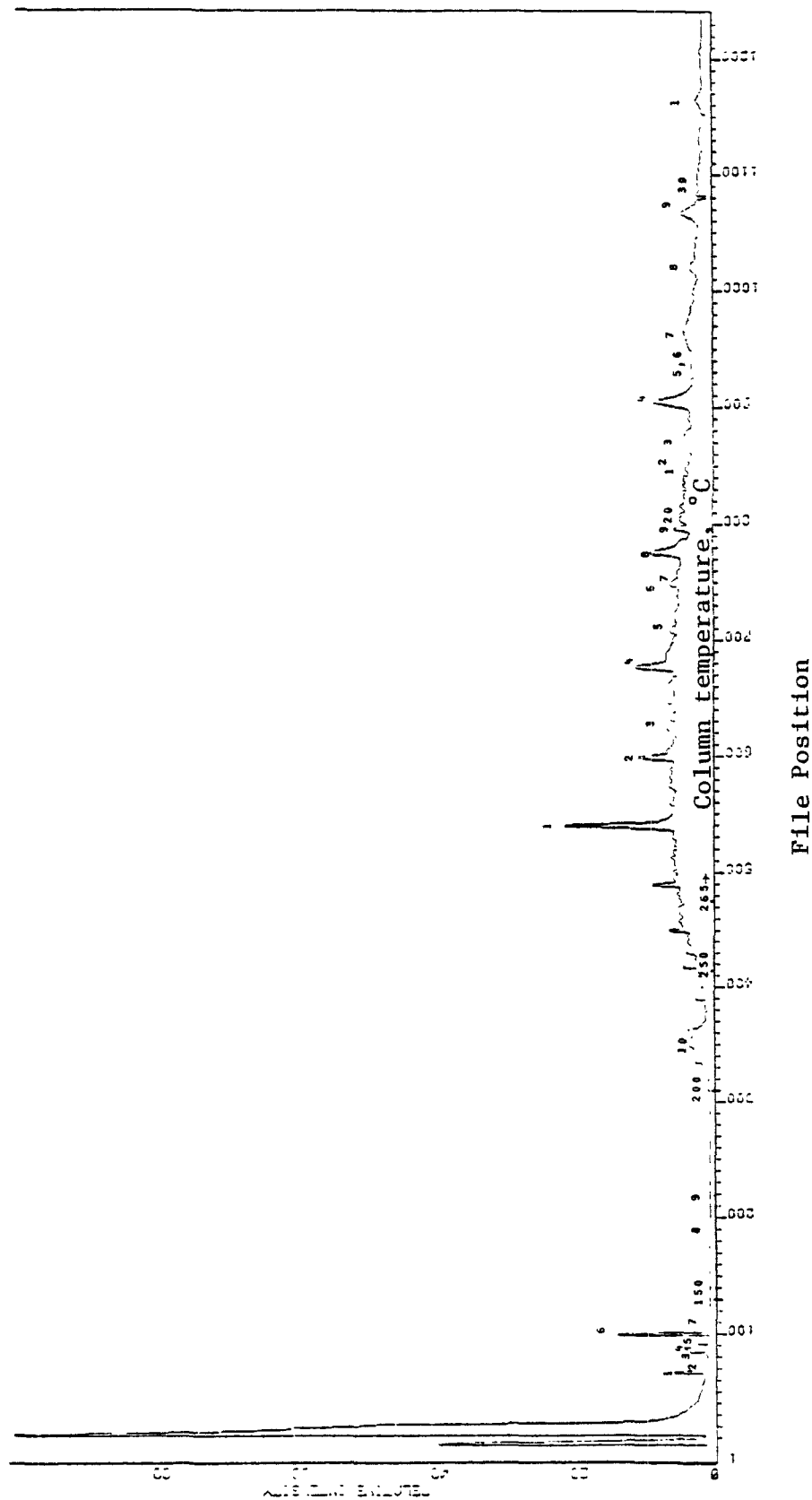


Figure D-3. Total ion current chromatogram of GC/MS/COMP analysis of paraffin fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

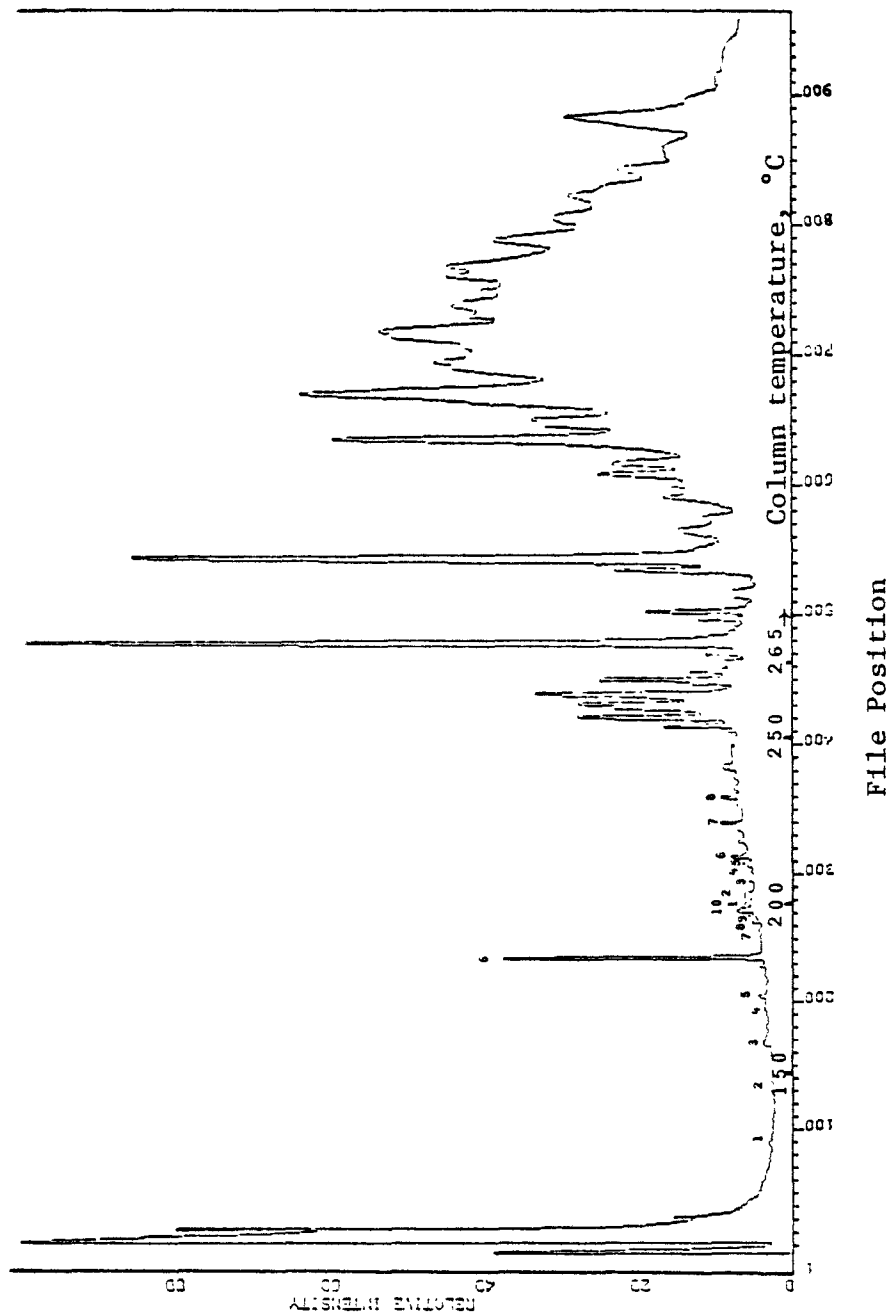


Figure D-4. Total ion current chromatogram of GC/MS/COMP analysis of base fraction of <1.7 μ air particulate collected in Kanawha Valley, WV (Trip 3, P1/L1)

APPENDIX E

VOLATILE AND VERY VOLATILE ORGANIC COMPOUNDS
IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA

Table E-1. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN FRONT ROYAL, VA (TRIP 1, P1/L4).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	12	70	3-methylpentane
2A	52	propane (tent.)	13	71	hexafluorobenzene (a#)
	52	isobutane (tent.)	14	72	n-hexane
	52	butene isomer	15	73	chloroform
3	53	n-butane	16	76	perfluorotoluene (a#)
	54	butene isomer	16A	78	methylcyclopentane
4	54	acetaldehyde	16B	82	benzene
	56	C ₅ H ₁₀ isomer (tent.)	16C	84	cyclohexane
5	57	isopentane	16D	85	C ₇ H ₁₆ isomer
6	58	acetone	16E	86	C ₇ H ₁₆ isomer
7	59	n-pentane	17	89	C ₈ H ₁₈ isomer
7A	60	diethyl ether	18	94	acetic acid
8	61	vinylidene chloride	19	103	toluene
9	61	methylene chloride	19A	107	C ₈ H ₁₈ isomer
10A	63	CS ₂	20	109	C ₈ H ₁₆ isomer
10B	65	C ₄ H ₈ O isomer	21	111	C ₈ H ₁₆ isomer
10C	67	C ₅ H ₁₀ isomer	22	113	C ₈ H ₁₆ isomer
11	68	2-methylpentane			

Table E-2. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN FRONT ROYAL, VA (TRIP 1, P2/L5).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	10	73	n-hexane
2A	52	C ₄ H ₈ isomer + propane (tent.)	10A	74	chloroform
3	53	n-butane	10B	75	C ₅ H ₁₀ O isomer
3A	54	C ₄ H ₈ isomer	11	77	perfluorotoluene (e%)
3B	55	acetaldehyde	12	79	methylcyclopentane
4	58	isopentane	13	83	benzene
4B	59	propanal	14	85	cyclohexane
4C	59	acetone	15	88	n-pentanal
4D	60	n-pentane	16A	92	n-heptane
4E	60	diethyl ether	16B	95	C ₇ H ₁₄ isomer
4F	61	vinylidene chloride	17	105	toluene
5	62	methylene chloride	17A	106	C ₈ H ₁₈ isomer (tent.)
6A	64	CS ₂	17B	109	C ₆ H ₁₂ O isomer
6B	67	C ₄ H ₆ O isomer	18	110	n-hexanal
7	68	2-methylpentane	18A	111	C ₈ H ₁₆ isomer
7A	70	n-butanal	19	113	n-octane
8	71	3-methylpentane	20	117	C ₈ H ₁₆ isomer (tent.)
9	72	hexafluorobenzene (e%)			

Table E-3. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN FRONT ROYAL, VA (TRIP 1, P3/L2).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	28	145	C ₁₀ H ₂₂ isomer
2A	54	C ₄ H ₈ isomer	28A	148	C ₁₀ H ₁₆ isomer
2B	56	n-butane	29	146	benzaldehyde
2C	57	acetaldehyde	29A	147	n-propylbenzene
2D	60	isopentane (tent.)	30	148	ethyltoluene isomer
3	61	acetone	30A	149	C ₈ H ₁₆ O isomer
4	63	diethyl ether	30B	149	phenol
5	64	vinylidene chloride	31	150	C ₁₁ H ₂₄ isomer
6	65	dichloromethane	31A	151	C ₁₀ H ₂₀ isomer
8	71	2-methylpentane	31B	151	C ₈ H ₁₆ O isomer
9	74	3-methylpentane + n-butanal	32	152	C ₁₁ H ₂₄ isomer
9A	75	C ₆ H ₁₂ isomer	33	153	n-octanal
10	76	hexafluorobenzene (e ₃)	34	154	1,2,4-trimethylbenzene
11	77	n-hexane	34A	155	C ₁₀ H ₂₀ isomer
12	78	chloroform	35	156	n-decane
13	79	ethyl acetate	35A	157	dichlorobenzene isomer (tent.)
14	81	perfluorotoluene (e ₃)	35B	159	C ₁₁ H ₂₄ isomer
14A	82	methylcyclopentane	35C	160	1,2,3-trimethylbenzene
15	87	benzene	36	160	C ₁₁ H ₂₄ isomer
15A	87	carbon tetrachloride	36A	162	indan
15B	88	cyclohexane	37	164	C ₄ -alkyl benzene + C ₁₂ H ₂₆ isomers
15C	90	C ₇ H ₁₄ isomer (tent.)	38	165	acetophenone
16	91	acetic acid	38A	166	cresol isomer
17	93	pentanal (tent.)	38B	166	C ₉ H ₁₈ O isomer
18	96	n-heptane	38C	168	sat. hydrocarbon
18A	101	C ₇ H ₁₄ isomer	38D	169	C ₄ -alkyl benzene isomer
19	109	toluene	38E	170	C ₁₁ H ₂₂ isomer
19A	110	C ₈ H ₁₈ isomer	38F	170	C ₄ -alkyl benzene isomer
19B	111	C ₈ H ₁₈ isomer	39	171	n-nonanal
19C	113	C ₈ H ₁₆ isomer	40	173	n-undecane
20	114	n-hexanal	40A	174	C ₁₁ H ₂₀ isomer (tent.)
20A	115	C ₈ H ₁₆ isomer	41	178	dimethylphenol isomer
21	117	n-octane	42	181	C ₂ -alkyl phenol isomer
22	119	tetrachloroethylene	43	183	C ₂ -alkyl phenol isomer
22A	123	C ₈ H ₁₆ isomer	43A	185	C ₅ -alkyl benzene isomer
22B	126	unsat. hydrocarbon	43B	185	C ₁₀ H ₂₀ O isomer
23	129	ethylbenzene	44	186	C ₃ -alkyl phenol isomer
23A	130	C ₉ H ₁₈ isomer	44A	187	naphthalene
24	131	xylene + C ₉ H ₂₀ isomers	45	188	n-decanal
24A	134	C ₉ H ₂₀ isomer	45A	189	C ₁₂ H ₂₄ isomer
24B	134	styrene	46	189	n-dodecane
25	135	o-xylene + n-heptanal	46A	190	C ₂ -alkyl phenol isomer
25A	136	C ₉ H ₂₀ isomer	46B	191	C ₃ -alkyl phenol isomer
25B	137	C ₉ H ₁₈ isomer	46C	193	C ₃ -alkyl phenol isomer
26	138	n-nonane	47	194	unknown
27	141	C ₁₀ H ₂₂ isomer			

(continued)

Table E-3. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
48	195	unknown	53	213	alkyl butyrate (BKG)
48A	201	C ₁₁ H ₂₂ O isomer	54	214	alkyl isobutyrate (BKG)
49	203	<u>n</u> -undecanal	54A	216	C ₆ -alkyl phenol
49A	204	C ₁₃ H ₂₆ isomer	55	217	<u>n</u> -tetradecane
50	204	<u>n</u> -tridecane	55A	228	C ₁₂ H ₂₄ O isomer (tent.)
50A	205	8-methylnaphthalene	56	229	C ₁₅ H ₃₀ isomer
51	206	unknown	57	230	<u>n</u> -pentadecane
52	211	C ₁₄ H ₃₀ isomer (tent.)	58	232	unknown

Table E-4. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 1, P3/L6).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	12B	69	methyl vinyl ketone
2A	52	C ₄ H ₈ isomer	13	70	3-methylpentane
3	53	<u>n</u> -butane	13A	70	methyl ethyl ketone
4	54	C ₄ H ₈ isomer	14	71	hexafluorobenzene (e ₃)
5	57	isopentane	15	72	<u>n</u> -hexane
6A	58	acetone	15A	73	chloroform
7	59	<u>n</u> -pentane	16	76	perfluorotoluene (e ₃)
8	61	vinylidene chloride	17	77	methylcyclopentane
9	61	methylene chloride	17A	81	C ₅ H ₁₀ O isomer (tent.)
11	63	CS ₂	18	82	benzene
12	67	2-methylpentane	19	84	cyclohexane
12A	69	<u>n</u> -butanal	19A	86	<u>n</u> -heptane (tent.)

Table E-5. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN FRONT ROYAL, VA (TRIP 1, P3/L6).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	28	131	xylene isomer
5	53	propane	29	133	C ₉ H ₂₀ isomer
5A	54	butene isomer	29A	134	C ₇ H ₁₄ O isomer
5B	54	n-butane	29B	134	n-heptaldehyde (tent.)
6	56	acetaldehyde	29C	135	styrene
6A	59	isopentane	30	136	o-xylene
7	61	acetone	30A	137	C ₉ H ₁₈ isomer
7A	65	dichloroethylene isomer (tent.)	31	138	n-nonane
8	65	dichloromethane	31A	140	C ₉ H ₁₈ isomer (tent.)
9A	71	C ₄ H ₆ O isomer	32	142	isopropylbenzene + C ₁₀ H ₂₂ isomer
10	72	2-methylpentane	33	145	C ₃ -alkyl cyclohexane + C ₁₀ H ₂₂ isomers
11	75	3-methylpentane	33A	146	C ₁₀ H ₁₆ isomer
11A	76	C ₆ H ₁₂ isomer	34	147	benzaldehyde
12	76	hexafluorobenzene (aF)	34A	148	n-propylbenzene
13	77	n-hexane	35	149	ethyltoluene isomer
14	78	chloroform	35A	150	C ₁₀ H ₂₂ isomer
15	82	perfluorotoluene (aF)	36	150	1,3,5-trimethylbenzene + phenol
15A	83	methylcyclopentane	36A	151	C ₁₁ H ₂₄ isomer
15B	85	1,1,1-trichloroethane	36B	152	C ₁₀ H ₂₂ isomer
15C	87	C ₆ H ₁₀ isomer	36C	152	o-ethyltoluene
16	88	benzene	37	154	n-octanal
16A	88	carbon tetrachloride (tent.)	38	155	1,2,4-trimethylbenzene
16B	89	cyclohexane	38A	156	C ₁₀ H ₂₀ isomer
17	90	acetic acid + C ₇ H ₁₆ isomer	39	157	n-decane
18	92	3-methylhexane	39A	158	dichlorobenzene isomer
18A	94	n-pentanal	39B	158	C ₄ -alkyl benzene isomer
19	95	C ₈ H ₁₈ isomer	39C	159	C ₁₀ H ₂₀ isomer
19A	96	C ₇ H ₁₄ isomer	39D	160	C ₄ -alkyl benzene isomer
20	97	n-heptane	40	161	1,2,3-trimethylbenzene
20A	100	C ₈ H ₁₈ isomer	40A	161	C ₁₁ H ₂₄ isomer
20B	103	methylcyclohexane	40B	163	indan
20C	104	C ₈ H ₁₈ isomer	40C	164	C ₁₀ H ₂₀ isomer
20D	105	C ₆ H ₁₂ O isomer	40D	165	C ₄ -alkyl benzene isomer
21	110	toluene	40E	165	C ₄ -alkyl benzene isomer
22	111	C ₈ H ₁₈ isomer	41	166	acetophenone
23	113	C ₈ H ₁₈ isomer	41A	166	C ₄ -alkyl benzene isomer
23A	114	C ₈ H ₁₆ isomer	41B	167	cresol isomer
24	115	n-hexanal	41C	167	C ₁₁ H ₂₄ isomer
24A	116	C ₈ H ₁₆ isomer	41D	168	C ₁₁ H ₂₂ isomer
25	118	n-octane	41E	168	C ₁₁ H ₂₄ isomer
26	119	tetrachloroethylene	41F	170	C ₄ -alkyl benzene isomer
26A	124	C ₉ H ₂₀ isomer	41G	170	C ₉ H ₁₈ O isomer
26B	126	C ₈ H ₁₆ + C ₉ H ₂₀ isomers	41H	171	C ₄ -alkyl benzene isomer
26C	128	C ₉ H ₁₈ isomer			
26D	128	C ₇ H ₁₄ O aldehyde isomer			
27	129	ethylbenzene			

(continued)

Table E-5. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
42	172	<u>n</u> -nonanal	49A	191	C ₃ -alkyl phenol isomer
42A	171	C ₁₁ H ₂₂ isomer	49B	193	C ₃ -alkyl phenol isomer
43	174	<u>n</u> -undecane	49C	198	C ₁₃ H ₂₈ isomer
43A	175	C ₄ -alkyl benzene isomer	50	204	<u>n</u> -undecanal
43B	176	C ₁₁ H ₂₂ isomer	51	205	<u>n</u> -tridecane
43C	177	C ₄ -alkyl benzene isomer	51A	205	β -methylnaphthalene
43D	177	tetramethylbenzene isomer	51B	206	unsat. hydrocarbon
43E	178	C ₁₂ H ₂₆ isomer	51C	208	α -methylnaphthalene
44	179	dimethylphenol isomer	52	213	alkyl butyrate
44A	181	C ₄ H ₇ -benzene + C ₅ -alkyl benzene isomers	53	215	alkyl butyrate
44B	181	C ₁₁ H ₂₂ isomer	53A	216	biphenyl
45	182	ethylphenol isomer	53B	217	C ₆ -alkyl phenol isomer
45A	183	C ₄ -alkyl benzene isomer	54	218	<u>n</u> -tetradecane
46	184	dimethylphenol isomer	54A	221	C ₂ -alkyl naphthalene isomer (tent.)
46A	185	C ₄ -alkyl benzene isomer	54B	230	C ₁₅ H ₃₀ isomer
47	186	C ₃ -alkyl phenol isomer	55	231	<u>n</u> -pentadecane
47A	186	C ₁₂ H ₂₄ isomer	56	233	unknown
47B	187	naphthalene	57	240	diethyl phthalate
48	188	<u>n</u> -decanal	57A	240	C ₁₆ H ₃₂ isomer
48A	189	C ₅ -alkyl benzene isomer	58A	240	<u>n</u> -hexadecane
49	190	<u>n</u> -dodecane	58B	240	benzophenone

Table E-6. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 2, P2/L3).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	49	CO ₂	24	109	C ₉ H ₂₀ isomer
2A	55	acetaldehyde	24A	111	C ₈ H ₁₆ isomer
2B	57	n-butane	25	112	n-octane
3	59	acetone	25A	113	C ₈ H ₁₆ isomer
3A	61	diethyl ether (tent.)	26	113	tetrachloroethylene
3B	62	dichloroethylene isomer	26A	117	C ₉ H ₂₀ isomer
4	63	dichloromethane	27	118	C ₉ H ₂₀ isomer
6	65	CS ₂	28	119	ethylcyclohexane or C ₈ H ₁₆ isomer
6A	69	C ₅ H ₁₀ isomer	28A	120	C ₉ H ₂₀ isomer
7	70	2-methylpentane	28B	120	C ₉ H ₁₈ isomer
7A	71	C ₃ H ₈ O isomer	28C	122	C ₉ H ₁₈ isomer
7B	71	C ₄ H ₈ O isomer	29	123	ethylbenzene
7C	72	3-methylpentane	29A	124	C ₉ H ₁₈ isomer
7D	72	C ₆ H ₁₂ isomer	29B	124	C ₉ H ₂₀ isomer
7E	73	methyl ethyl ketone	30	125	xylene isomer
8	73	hexafluorobenzene (a ₂)	30A	125	C ₉ H ₂₀ isomer
9	74	n-hexane	31	127	C ₉ H ₂₀ isomer
10	75	chloroform	31A	127	C ₇ H ₁₄ O isomer (tent.)
10A	76	ethyl acetate	32	128	C ₉ H ₂₀ isomer
10B	77	C ₆ H ₁₂ isomer	32A	129	styrene
11	78	perfluorotoluene (a ₂)	32B	129	C ₉ H ₁₈ isomer
12	79	methylcyclopentane	33	130	o-xylene
12A	80	1,2-dichloroethane (tent.)	33A	131	C ₉ H ₁₈ isomer
13	81	1,1,1-trichloroethane	34	132	n-nonane
14	83	benzene	34A	134	C ₉ H ₁₈ isomer
14A	84	carbon tetrachloride	35	135	C ₁₀ H ₂₂ isomer
14B	85	cyclohexane	36	136	C ₁₀ H ₂₂ isomer + isopropylbenzene
15	85	2-methylhexane	37	137	C ₁₀ H ₂₂ isomer
15A	86	2,3-dimethylpentane	37A	138	C ₁₀ H ₂₀ isomer
16	87	3-methylhexane	38	139	C ₁₀ H ₂₂ + C ₃ -alkyl cyclohexane isomers
16A	88	pentanal	39	140	C ₁₀ H ₁₆ isomer
16B	89	C ₇ H ₁₄ isomer	40	141	benzaldehyde
17	90	trichloroethylene	40A	141	n-propylbenzene
17A	90	C ₈ H ₁₈ isomer (tent.)	40B	142	C ₁₀ H ₂₀ isomer
18	92	n-heptane	41	143	ethyltoluene isomer
18A	93	C ₇ H ₁₄ isomer	41A	144	1,3,5-trimethylbenzene
18B	96	C ₈ H ₁₈ isomer	42	144	C ₁₁ H ₂₄ isomer
19	97	methylcyclohexane	42A	145	phenol
20	97	acetic acid	42B	145	C ₁₀ H ₂₂ isomer
20A	98	C ₇ H ₁₄ O isomer (tent.)	43	146	o-ethyltoluene
20B	101	C ₈ H ₁₆ isomer	44	147	sat. hydrocarbon
21	103	toluene	45	147	C ₁₀ H ₁₆ isomer
22	105	C ₈ H ₁₈ isomer	45A	148	C ₁₀ H ₂₀ isomer
23	106	C ₈ H ₁₈ isomer			
23A	107	C ₈ H ₁₆ isomer			
23B	108	C ₈ H ₁₆ isomer			

(continued)

Table E-6. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
46	148	1,2,4-trimethylbenzene	60A	175	C ₄ H ₇ -benzene isomer (tent.)
46A	149	C ₁₀ H ₂₀ isomer	60B	176	C ₄ -alkyl benzene isomer
47	150	n-decane	60C	176	C ₅ -alkyl benzene isomer
47A	151	dichlorobenzene isomer	61	176	C ₂ -alkyl phenol isomer
48	151	C ₁₁ H ₂₄ isomer (tent.)	61A	177	C ₅ -alkyl benzene isomer
48A	152	C ₄ -alkyl benzene isomer	61B	179	C ₂ -alkyl phenol isomer
48B	153	C ₄ -alkyl benzene isomer	62	179	C ₃ -alkyl phenol isomer
48C	153	1,2,3-trimethylbenzene	63	181	naphthalene + C ₁₂ H ₂₄ isomer
49	154	C ₄ -alkyl benzene + C ₁₁ H ₂₄ isomers	64	183	n-dodecane
50	155	C ₁₁ H ₂₄ isomer	64A	183	C ₁₃ H ₂₆ isomer
50A	156	C ₁₀ H ₁₆ isomer	65	184	C ₃ -alkyl phenol isomer
50B	156	indan	66	187	unknown
51	157	C ₁₁ H ₂₄ isomer	66A	189	C ₁₃ H ₂₆ isomer
51A	157	C ₁₀ H ₂₀ isomer	66B	195	C ₁₃ H ₂₆ isomer
52	158	C ₁₁ H ₂₄ isomer	67	196	n-tridecane
52A	158	C ₄ -alkyl benzene isomer	67A	197	β-methylnaphthalene
53	159	acetophenone	67B	198	C ₁₃ H ₂₆ isomer
53A	160	cresol isomer	67C	199	α-methylnaphthalene
53B	160	C ₁₁ H ₂₄ + C ₄ -alkyl benzene isomers	67D	204	C ₁₃ H ₂₆ isomer
54	161	C ₁₁ H ₂₄ isomer	68	205	alkyl butyrate
54A	161	C ₁₁ H ₂₂ isomer	69	207	alkyl butyrate
54B	163	C ₄ -alkyl benzene isomer	69A	208	C ₁₂ H ₂₄ O isomer
54C	163	C ₁₁ H ₂₂ isomer	69B	208	biphenyl (tent.)
55	164	C ₄ -alkyl benzene isomer	69C	209	C ₆ -alkyl phenol isomer
55A	165	C ₄ H ₇ -benzene isomer	70	209	C ₁₄ H ₂₈ isomer
56	165	n-nonanal	71	210	sat. hydrocarbon
56A	166	C ₁₁ H ₂₂ isomer	71A	212	C ₂ -alkyl naphthalene isomer
57	167	n-undecane	73	219	unsat. hydrocarbon
57A	167	C ₅ -alkyl benzene isomer	73A	221	C ₁₃ H ₂₆ O isomer (tent.)
57B	168	C ₁₁ H ₂₂ isomer	73B	222	C ₁₅ H ₃₀ isomer
58	170	C ₄ -alkyl benzene isomer	74	223	n-pentadecane
59	172	dimethylphenol isomer	75	225	unknown
59A	173	C ₅ -alkyl benzene isomer	76	232	diethyl phthalate
59B	173	C ₄ H ₇ -benzene isomer	76A	234	C ₁₄ H ₂₈ O isomer
60	174	C ₂ -alkyl phenol isomer	77A	236	C ₁₆ H ₃₂ isomer
			77B	240	C ₁₅ H ₃₀ O isomer (tent.)
			78	240	n-heptadecane

Table E-7. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 2, P3/L5).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	28C	129	styrene
4	51	n-propane (tent.)	29	130	o-xylene + C ₉ H ₂₀ isomer
4A	51	butene isomer	29A	131	C ₉ H ₁₈ isomer (tent.)
5	52	n-butane	30	132	n-nonane
6	53	acetaldehyde	31	136	C ₁₀ H ₂₂ isomer
6A	55	isopentane	32	139	C ₁₀ H ₂₂ isomer
7	58	acetone	33	140	C ₁₀ H ₁₆ isomer
7A	60	diethyl ether (tent.)	34	141	benzaldehyde
8	61	vinylidene chloride	34A	143	ethyltoluene isomer
9	62	dichloromethane	34B	144	C ₈ H ₁₆ O isomer
10A	66	C ₄ H ₈ O isomer	34C	144	phenol + C ₃ -alkyl benzene isomer
11	68	cyclopentane	35	145	C ₁₁ H ₂₄ isomer
11A	68	2-methylpentane	35A	146	C ₃ -alkyl benzene isomer
11B	69	methyl isopropyl ketone (tent.)	36	147	C ₁₀ H ₂₂ isomer
12	70	n-butanal	36A	148	C ₁₁ H ₂₄ isomer
12A	71	3-methylpentane	37	149	n-octanal
13	72	hexafluorobenzene (aF)	37A	149	trimethylbenzene isomer
14	73	n-hexane	38	150	n-decane
14A	74	chloroform	38A	151	C ₁₁ H ₂₄ isomer
15	75	ethyl acetate	38B	152	C ₁₀ H ₂₀ isomer (tent.)
16	77	perfluorotoluene (aF)	38C	154	C ₁₁ H ₂₄ isomer
17	78	methylcyclopentane	39	156	sat. hydrocarbon
18	83	benzene	40	159	C ₁₁ H ₂₄ isomer
18A	84	carbon tetrachloride	41	160	acetophenone
19	84	cyclohexane	41A	161	cresol isomer
19A	85	2-methylhexane	41B	162	C ₁₂ H ₂₆ isomer (tent.)
19B	86	2,3-dimethylpentane	41C	164	C ₄ -alkyl benzene isomer
20	87	3-methylhexane + C ₇ H ₁₄ isomer	41D	165	C ₉ H ₁₈ O isomer
20A	88	acetic acid (tent.)	42	166	n-nonanal
21	90	C ₈ H ₁₈ isomer	42A	167	C ₁₁ H ₂₂ isomer
22	91	n-heptane	43	168	n-undecane
22A	93	C ₇ H ₁₄ isomer (tent.)	44	173	dimethylphenol isomer
22B	96	C ₈ H ₁₈ isomer	45	176	C ₂ -alkyl phenol isomer
23	97	methylcyclohexane	45A	178	C ₂ -alkyl phenol isomer
23A	99	C ₈ H ₁₈ isomer	45B	179	unsat. hydrocarbon
24	104	toluene	46	180	C ₃ -alkyl phenol isomer
24A	105	C ₈ H ₁₈ isomer	46A	181	naphthalene (tent.)
24B	107	C ₈ H ₁₈ isomer	47	182	n-decanal
25	109	n-nexanal (tent.) + C ₈ H ₁₆ isomer	48	183	n-dodecane
26	112	n-octane	48A	185	C ₃ -alkyl phenol isomer
27	113	tetrachloroethylene	48B	186	C ₁₂ H ₂₄ isomer
27A	123	ethylbenzene	48C	187	C ₃ -alkyl phenol isomer
28	125	xylene isomer	48D	191	unsat. hydrocarbon
28A	126	C ₉ H ₂₀ isomer (tent.)	48E	195	C ₁₁ H ₂₂ O isomer
28B	128	C ₇ H ₁₄ O isomer (tent.)	49	197	n-undecanal

(continued)

Table E-7. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
50	198	<u>n</u> -tridecane	53B	222	C ₁₃ H ₂₆ O isomer
50A	198	β -methylnaphthalene	54	223	C ₁₅ H ₃₀ isomer
50B	201	α -methylnaphthalene	55	224	<u>n</u> -pentadecane
50C	204	unsat. hydrocarbon	56	226	unknown
50D	205	unsat. hydrocarbon	57	233	diethyl phthalate
51	208	alkyl butyrate	57A	235	C ₁₆ H ₃₂ isomer
51A	209	C ₁₂ H ₂₄ O isomer	58A	236	<u>n</u> -hexadecane (tent.)
51B	211	unsat. hydrocarbon	58B	240	benzophenone
52	212	<u>n</u> -tetradecane	58C	240	C ₁₅ H ₃₀ O isomer
53	217	unknown	58D	240	C ₁₇ H ₃₄ isomer
53A	221	unsat. hydrocarbon	58E	240	<u>n</u> -heptadecane

Table E-8. VERY VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 3, P1/L9).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	8	61	acetone
3A	53	propane	8A	64	diethyl ether (tent.)
3B	53	propylene	9	65	methylene chloride
4	54	isobutane	10A	67	CS ₂
4A	55	C ₄ H ₈ isomer	12	72	2-methylpentane
5	56	acetaldehyde	13	75	3-methylpentane
5A	57	C ₄ H ₈ isomer	14	76	hexafluorobenzene (a ₁)
6	58	<u>n</u> -butane	15	77	<u>n</u> -hexane
7	60	isopentane	15A	78	chloroform

Table E-9. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR
IN FRONT ROYAL, VA (TRIP 3, P2/L8).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	48	CO ₂	39B	111	C ₆ H ₁₂ O isomer
3A	51	propane (tent)	40	112	hexanal
5	53	C ₄ H ₁₀ isomer	40A	113	C ₈ H ₁₆ isomer
6	55	acetaldehyde	41	114	n-octane
7	56	n-butane	41A	115	C ₈ H ₁₆ isomer
8	58	isopentane	42	116	tetrachloroethylene
9	59	acetone	43	118	C ₈ H ₁₆ isomer
10	60	n-pentane	43A	119	C ₉ H ₂₀ isomer
11	61	diethyl ether	43B	121	C ₉ H ₂₀ isomer
12	62	Background peak	43C	121	C ₈ H ₁₆ isomer
13	63	methylene chloride	44	122	C ₉ H ₂₀ isomer + ethylcyclohexane
16	67	C ₆ H ₁₄ isomer (tent)	44A	123	C ₉ H ₁₈ isomer
16A	69	C ₅ H ₁₀ isomer	45	126	ethylbenzene
17	70	2-methylpentane	45A	126	C ₉ H ₁₈ isomer
18	72	3-methylpentane	45B	127	C ₉ H ₂₀ isomer
19	74	hexafluorobenzene (e3)	46	127	xylene isomer
20	75	n-hexane	46A	128	C ₉ H ₂₀ isomer
20A	76	chloroform	47	129	C ₉ H ₂₀ isomer
21	77	methyl ethyl ketone (tent)	47A	130	C ₇ H ₁₄ O isomer
21A	78	ethyl acetate (tent)	48	131	styrene
22	79	perfluorotoluene (e3)	48A	131	n-heptanal
23	80	methylcyclopentane	49	132	o-xylene
24	81	1,1,1-trichloroethane	49A	133	C ₉ H ₁₈ isomer
24A	83	C ₇ H ₁₄ isomer	50	134	n-nonane
24B	84	C ₆ H ₁₀ isomer	50A	135	C ₁₀ H ₂₂ isomer
25	85	benzene	50B	137	C ₉ H ₁₈ isomer
25A	86	carbon tetrachloride (tent)	51	138	C ₁₀ H ₂₂ isomer + isopropyl- benzene
26	87	cyclohexane	52	139	C ₈ H ₁₆ O isomer
27	87	2-methylhexane	53	141	C ₁₀ H ₂₂ isomer
27A	88	2,3-dimethylpentane	54	142	C ₁₀ H ₁₆ isomer
27B	88	acetic acid	55	143	benzaldehyde
28	89	3-methylhexane	56	144	n-propylbenzene
29	91	n-pentanal	57	145	ethyltoluene isomer
29A	91	C ₇ H ₁₄ isomer	57A	146	phenol
30	92	C ₈ H ₁₈ isomer + trichloro- ethylene	57B	146	1,3,5-trimethylbenzene
31	94	n-heptane	58	147	C ₁₀ H ₂₂ isomer
32	95	C ₇ H ₁₂ isomer	59	148	o-ethyltoluene
33	97	unsat. hydrocarbon	59A	149	C ₁₀ H ₂₂ isomer
34	99	methylcyclohexane	59B	149	C ₁₁ H ₂₄ isomer
35	101	C ₈ H ₁₈ + C ₆ H ₁₂ O isomers	60	150	n-octanal isomer (tent)
36	105	C ₈ H ₁₈ isomer	60A	151	C ₁₀ H ₂₀ isomer
37	106	toluene	61	151	1,2,4-trimethylbenzene
38	108	C ₈ H ₁₈ isomer	61A	152	C ₁₀ H ₂₀ isomer
39	109	C ₈ H ₁₈ isomer	62	153	n-decane
39A	111	C ₈ H ₁₆ isomer			

(continued)

Table E-9. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
62A	154	dichlorobenzene isomer	72D	179	C ₅ -alkyl benzene isomer
62B	154	C ₄ -alkyl benzene isomer	72E	179	C ₂ -alkyl phenol isomer
62C	155	C ₁₁ H ₂₄ isomer	73	180	C ₄ -alkyl benzene + C ₁₂ H ₂₆ isomers
62D	156	C ₄ -alkyl benzene isomer	73A	181	C ₁₂ H ₂₆ isomer
63	156	1,2,3-trimethylbenzene	73B	183	C ₅ -alkyl benzene + C ₁₂ H ₂₄ isomers
63A	157	C ₁₁ H ₂₄ isomer	73C	183	C ₂ -alkyl phenol isomer
63B	159	indan	73D	184	C ₂ -alkyl phenol isomer
63C	160	C ₄ -alkyl cyclohexane isomer	74	185	naphthalene + <u>n</u> -decanal
64	161	C ₄ -alkyl benzene isomer	74A	186	C ₁₂ H ₂₄ isomer
64A	161	C ₄ -alkyl benzene isomer	75	187	<u>n</u> -dodecane
65	162	acetophenone + C ₄ -alkyl benzene isomer	75A	189	C ₁₃ H ₂₈ isomer
65A	163	cresol isomer	75B	190	C ₃ -alkyl phenol isomer
65B	163	C ₁₁ H ₂₂ isomer	76	192	unknown
66	164	C ₁₁ H ₂₄ isomer	76A	197	C ₁₄ H ₃₀ isomer
66A	164	C ₄ -alkyl benzene isomer	76B	199	unsat. hydrocarbon
66B	165	C ₁₀ H ₁₈ isomer	77	200	<u>n</u> -undecanal
67	166	C ₁₁ H ₂₄ isomer	78	201	<u>n</u> -tridecane
67A	167	C ₄ -alkyl benzene isomer	78A	202	β -methylnaphthalene
68	168	C ₄ -alkyl benzene isomer	79	204	unknown
69	169	<u>n</u> -nonanal	79A	204	α -methylnaphthalene
69A	170	C ₁₁ H ₂₂ isomer	80	215	<u>n</u> -tetradecane
70	171	<u>n</u> -undecane	80A	228	unsat. hydrocarbon
70A	172	C ₄ -alkyl benzene isomer	80B	229	<u>n</u> -pentadecane
70B	172	C ₁₁ H ₂₂ isomer	80C	230	C ₁₅ H ₃₀ isomer
70C	174	C ₄ -alkyl benzene isomer	81	232	unknown
71	175	C ₁₂ H ₂₄ isomer	81A	237	unsat. hydrocarbon
72	176	C ₂ -alkyl phenol isomer	81B	238	diethyl phthalate
72A	177	C ₅ -alkyl benzene isomer	81C	239	C ₁₆ H ₃₄ isomer
72B	178	C ₅ -alkyl benzene + C ₄ H ₇ benzene isomers	82A	240	C ₁₆ H ₃₄ isomer

Table E-10. VOLATILE ORGANIC COMPOUNDS IDENTIFIED IN AMBIENT AIR IN FRONT ROYAL, VA (TRIP 3, P2/L9).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	47	CO ₂	24A	110	C ₈ H ₁₆ isomer
3	52	C ₄ H ₁₀ isomer (tent)	25	110	C ₈ H ₁₈ isomer
3A	53	acetaldehyde	25A	111	C ₈ H ₁₆ isomer
3B	55	SO ₂	25B	113	C ₈ H ₁₆ isomer
3C	57	isopentane	26	113	n-octane
4	59	acetone	26A	114	C ₈ H ₁₆ isomer
4A	60	n-pentane	27	115	tetrachloroethylene
4B	61	diethyl ether	27A	115	C ₈ H ₁₆ isomer
4C	61	Background peak	27B	117	C ₉ H ₂₀ isomer
5	62	methylene chloride	28	119	C ₉ H ₂₀ isomer
6A	64	CS ₂	28A	120	C ₈ H ₁₆ isomer
6B	68	C ₅ H ₁₀ isomer	29	121	C ₉ H ₂₀ isomer
7	69	2-methylpentane	29A	122	C ₉ H ₁₈ isomer
8	71	3-methylpentane	30	124	ethylbenzene
8A	72	C ₆ H ₁₂ isomer	30A	125	C ₉ H ₁₈ isomer
9	73	hexafluorobenzene (e#)	31	126	xylene
10	74	n-hexane	31A	126	C ₉ H ₂₀ isomer
10A	74	chloroform	32	127	C ₉ H ₂₀ isomer
10B	77	C ₆ H ₁₂ isomer	32A	128	C ₇ H ₁₄ ⁰ isomer (tent)
11	78	perfluorotoluene (e#)	33	129	styrene
12	79	methylcyclopentane	33A	129	C ₉ H ₁₈ isomer
12A	81	1,1,1-trichloroethane	34	130	o-xylene
13	84	benzene	34A	131	C ₉ H ₁₈ isomer
13A	85	carbon tetrachloride	35	132	n-nonane
13B	85	cyclohexane	35A	134	C ₁₀ H ₂₀ isomer
14	86	2-methylhexane	35B	135	C ₉ H ₁₈ isomer
14A	87	2,3-dimethylpentane	36	136	isopropylbenzene + C ₁₀ H ₂₂ isomer
15	88	3-methylhexane	37	137	C ₁₀ H ₂₂ isomer
15A	89	acetic acid	37A	138	C ₉ H ₁₆ isomer (tent)
16	90	C ₇ H ₁₄ isomer	37B	138	C ₁₀ H ₂₂ isomer
16A	90	C ₇ H ₁₄ isomer	38	139	C ₁₀ H ₂₂ + C ₃ -alkyl cyclohexane isomer
17	91	trichloroethylene + C ₈ H ₁₈ isomer	38A	140	C ₁₀ H ₁₆ isomer
18	93	n-heptane	39	141	benzaldehyde
18A	94	C ₇ H ₁₄ isomer	40	142	n-propylbenzene
18B	96	C ₇ H ₁₄ isomer	41	143	ethyltoluene isomer
18C	97	C ₈ H ₁₈ isomer	41A	144	C ₁₀ H ₂₂ isomer
19	98	methylcyclohexane	42	144	1,3,5-trimethylbenzene
19A	99	C ₈ H ₁₈ isomer	42A	145	C ₁₀ H ₂₂ isomer
19B	100	C ₆ H ₁₂ ⁰ isomer	42B	145	C ₁₀ H ₂₀ isomer
20	100	C ₈ H ₁₈ isomer	43	146	o-ethyltoluene
20A	101	C ₈ H ₁₆ isomer	43A	147	C ₁₁ H ₂₄ isomer
21	104	C ₈ H ₁₈ isomer	43B	148	C ₁₀ H ₂₀ isomer
22	105	toluene	43C	148	n-octanal
23	106	C ₈ H ₁₈ isomer	43D	149	C ₃ H ₅ -benzene isomer
24	108	C ₈ H ₁₈ isomer			

continued

Table E-10. (cont'd.)

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
44	149	1,2,4-trimethylbenzene	54B	172	C ₁₁ H ₂₀ isomer
44A	150	C ₁₀ H ₂₀ isomer	54C	173	C ₅ -alkyl benzene isomer
45	151	n-decane	54D	174	C ₅ -alkyl benzene isomer
45A	152	dichlorobenzene isomer	54E	175	C ₄ H ₇ -benzene isomer
45B	152	C ₄ -alkyl benzene isomer	54F	175	C ₅ -alkyl cyclohexane isomer
45C	153	C ₁₀ H ₂₀ isomer	54G	176	C ₅ -alkyl benzene isomer
45D	154	C ₄ -alkyl benzene isomer	55	177	C ₁₂ H ₂₆ + C ₄ -alkyl benzene isomers
46	154	1,2,3-trimethylbenzene	55A	177	C ₅ -alkyl benzene isomer
46A	155	C ₁₁ H ₂₄ isomer	55B	178	C ₄ alkyl benzene + C ₁₂ H ₂₆
46B	156	C ₁₁ H ₂₄ isomer	55C	179	C ₅ -alkyl benzene isomer
46C	157	indan	55D	180	C ₁₂ H ₂₄ + alkyl benzene isomers
46D	158	C ₄ -alkyl cyclohexane isomer	56	182	naphthalene
46E	158	C ₁₁ H ₂₂ + C ₄ -alkyl benzene isomers	56A	182	n-decanal
47	159	C ₄ -alkyl benzene isomer	56B	183	C ₁₂ H ₂₄ isomer
48	160	acetophenone + C ₄ -alkyl benzene isomer	56C	183	C ₅ -alkyl benzene isomer
48A	161	C ₁₁ H ₂₄ isomer	57	184	n-dodecane
48B	162	C ₁₁ H ₂₂ isomer	57A	185	C ₅ -alkyl benzene isomer
49	162	C ₄ -alkyl benzene isomer	57B	186	C ₁₃ H ₂₈ isomer
49A	163	C ₁₁ H ₂₄ isomer	57C	187	C ₆ -alkyl benzene isomer (tent)
50	164	C ₄ -alkyl benzene isomer	57D	190	C ₁₃ H ₂₆ isomer
50A	164	C ₁₁ H ₂₂ isomer	57E	192	C ₁₃ H ₂₈ isomer
50B	165	C ₄ H ₇ -benzene isomer (tent)	58	198	n-tridecane
51	165	C ₄ -alkyl benzene isomer	58A	199	β-methylnaphthalene
52	166	n-nonanal	58B	201	α-methylnaphthalene
52A	166	C ₄ -alkyl benzene isomer	58C	206	biphenyl (tent)
52B	167	C ₁₁ H ₂₂ isomer	59	208	n-tetradecane
53	168	n-undecane	59A	210	C ₁₄ H ₂₈ isomer
53A	168	C ₄ -alkyl benzene isomer	59B	216	C ₁₆ H ₃₄ isomer
53B	169	C ₁₁ H ₂₂ isomer	59C	217	unsat. hydrocarbon
53C	169	C ₅ -alkyl benzene isomer	59D	220	n-pentadecane
53D	170	C ₄ -alkyl benzene isomer	59E	221	C ₁₅ H ₃₀ isomer
54	171	tetramethylbenzene isomer	60	239	C ₁₆ H ₃₄ isomer
54A	172	C ₁₂ H ₂₆ isomer			

APPENDIX F

SEMIVOLATILE COMPOUNDS IDENTIFIED IN AIR PARTICULATE
COLLECTED IN SHENANDOAH VALLEY, VA

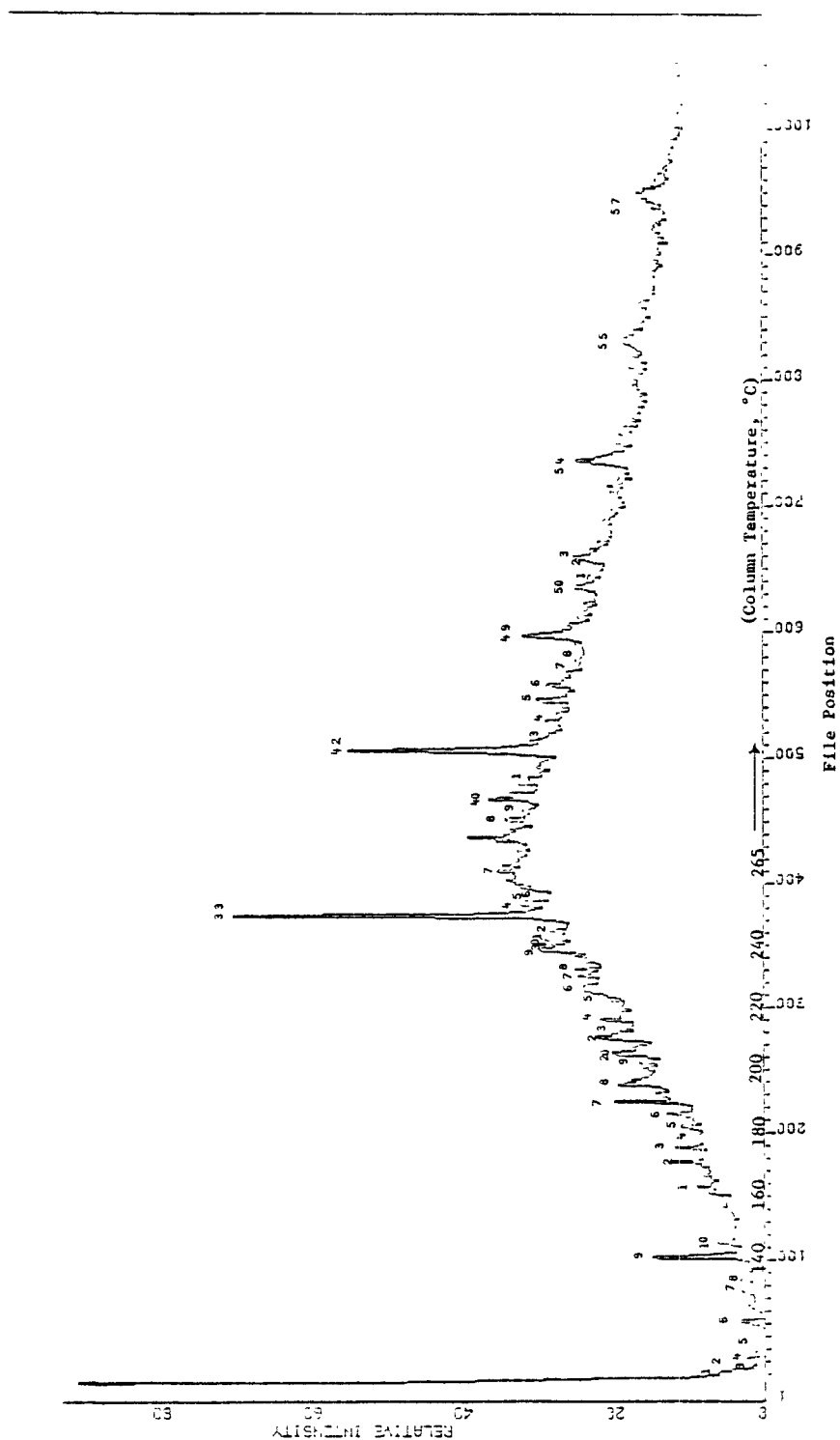


Figure F-1. Total ion current chromatogram of gc/ms/comp analysis of methanol extract of < 1.7 μ air particulate collected in Front Royal, VA (Trip 3, P1/L4).

Table F-1. COMPOUNDS IDENTIFIED IN METHANOL EXTRACT OF <1.7 μ FRACTION OF AIR PARTICULATE COLLECTED IN FRONT ROYAL, VA (TRIP 3, P1/L4).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	100-107	dichloromethane (solvent)	28	232	a phthalate (bkg.)
2	104-106	toluene (solvent)	29	238	naphthalic anhydride
3	108	benzaldehyde	30	239	C ₂ alkyl C ₁₈ H ₁₂ isomer ³ (tent.)
4	108.5	phenol	31	241	methylphenylindole isomer (tent.)
5	113	methylacetophenone isomer (tent.)	32	244	C ₁₆ H ₁₀ isomer ⁴
6	120.5	unknown	33	249	pyrene + pyrene-d ₁₀ (ext. std.)
7	129	naphthalene (tent.)	34	252	Si compd. (bkg.)
8	134.5	benzothiazole (tent.)	35	254	Si compd. (bkg.)
9	140-142	unknown	36	255	Si compd. (bkg.)
10	145	methylnaphthalene (tent.) + phthalic anhydride	37	265	Si compds. (bkg.) + phthalates (bkg.)
11	170.5	(C ₄ H ₉) ₂ benzoquinone isomer (tent.) + Si compd. (bkg.)	38	265	C ₁₈ H ₁₀ isomer ⁵
12	171	dibenzofuran (tent.)	39	265	C ₁₈ H ₁₄ isomer ⁶
13	175	unknown	40	265	C ₁₈ H ₁₂ isomer ³ + C ₁₈ H ₁₀ isomer (tent.)
14	177	di-butylcresol isomer (bkg.)	41	265	benzanthrone
15	181	C ₂ alkyl biphenyl isomer + Si compd. (bkg.)	42	265	a phthalate (bkg.)
16	185	a phthalate (bkg.)	43	265	C ₁₉ H ₁₄ isomer ⁷
17	189	unknown	44	265	C ₁₉ H ₁₂ isomer ⁸ (tent.)
18	195	4-hydroxy-3,5-dimethoxybenz- aldehyde	45	265	bkg.
19	202	unknown	46	265	unknown
20	204	methylxanthene isomer (tent.)	47	265	C ₂ alkyl C ₁₈ H ₁₂ isomer ³ (tent.)
21	207	methylxanthene isomer (tent.)	48	265	C ₂ alkyl C ₁₈ H ₁₀ isomer (tent.)
22	211	C ₁₄ H ₁₀ isomer(s) ¹	49	265	C ₂₀ H ₁₂ isomer ⁹
23	212	phenothiazine (tent.)	50	265	C ₂₀ H ₁₂ isomer ⁹
24	216	C ₂ alkyl xanthene	51	265	C ₂₀ H ₁₂ isomer ⁹ + C ₂ alkyl C ₁₈ H ₁₀ isomer
25	224	9-fluorenone (tent.)	52	265	C ₃ alkyl C ₁₈ H ₁₂ isomer ³ (tent.)
26	225	C ₁₅ H ₁₂ isomer ² (tent.)	53	265	C ₂₀ H ₁₂ isomer ⁹ (tent.)
27	231	unknown	54	265	C ₁₉ H ₁₄ isomer ⁷ (tent.)
			55	265	bkg.
			56	265	C ₂₂ H ₁₂ isomer ¹⁰
			57	265	C ₂₂ H ₁₂ isomer ¹⁰

Notes:

¹C₁₄H₁₀ isomers include anthracene, phenanthrene, and diphenyl acetylene.

²C₁₅H₁₂ isomers include methylphenanthrene and methylanthracene.

³C₁₈H₁₂ isomers include chrysene, benzophenanthrene isomers, triphenylene, naphthalene, and benzanthracene isomers.

⁴C₁₆H₁₀ isomers include pyrene, fluoranthene, and diphenyldiacetylene.

⁵C₁₈H₁₀ isomers include 1,10-benzfluoranthene and 3,4-cyclopentapyrene.

⁶C₁₈H₁₄ isomers include terphenyl isomers, styrylnaphthalene isomers, and dihydrobenzanthracene isomers.

⁷C₁₉H₁₄ isomers include methyltriphenylene isomers, methylbenzanthracene isomers, methylchrysene isomers, methylbenzophenanthrene isomers, and 9-phenylfluorene.

⁸C₁₉H₁₂ isomers include methyl-1,10-benzfluoranthene isomers.

⁹C₂₀H₁₂ isomers include perylene, benzpyrene isomers, and benzfluoranthene isomers.

¹⁰C₂₂H₁₂ isomers include 1,12-benzperylene, anthanthrene, and 2,3-o-phenyleneperylene.

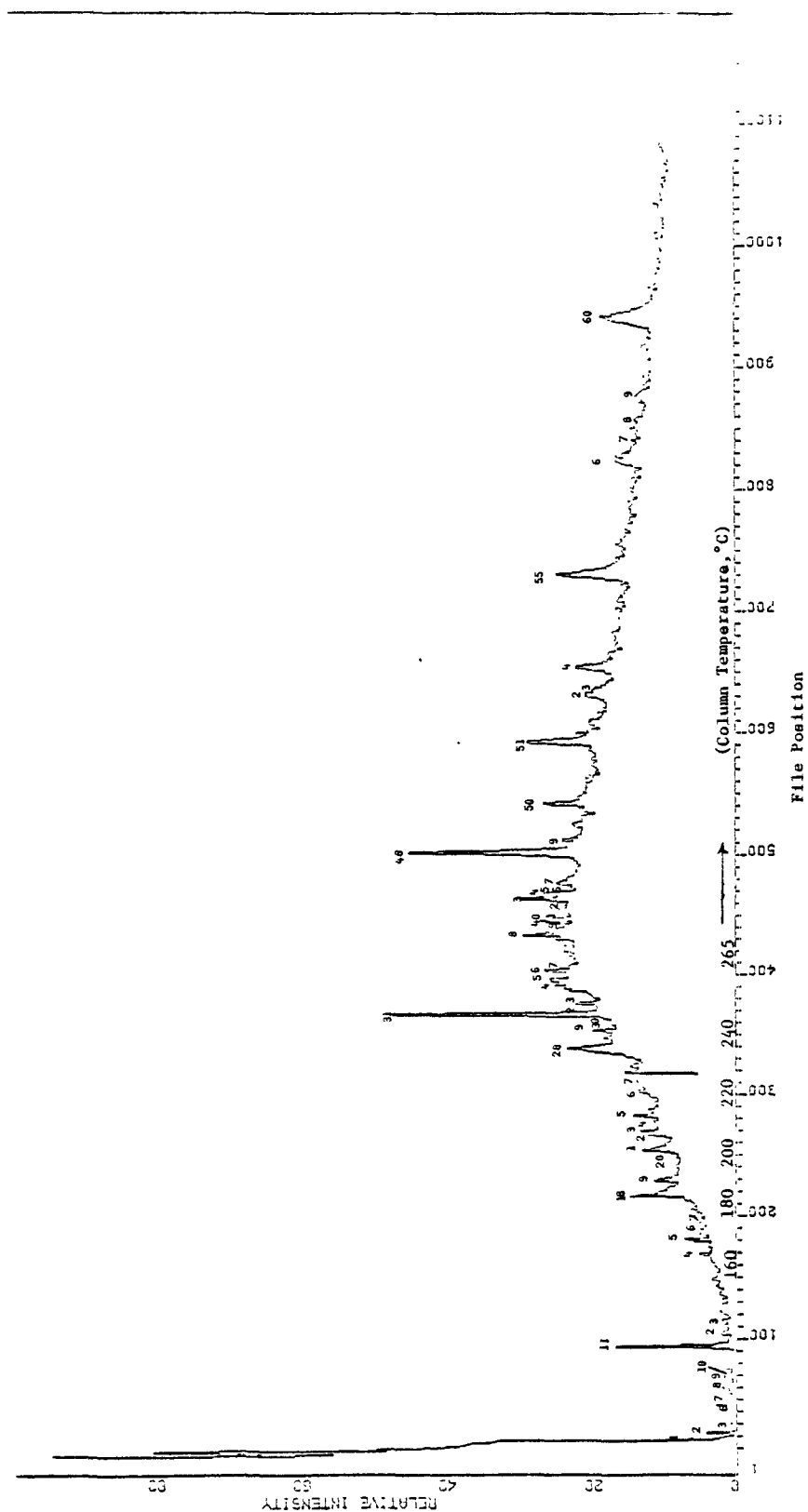


Figure F-2. Total ion current chromatogram of gc/ms/comp analysis of toluene extract of < 1.7 μ air particulate collected in Front Royal, VA (Trip 3, P1/L4).

Table F-2. COMPOUNDS IDENTIFIED IN TOLUENE EXTRACT OF <1.7 μ
FRACTION OF AIR PARTICULATE COLLECTED IN FRONT ROYAL,
VA (TRIP 3, P1/L4).

Chromato- graphic Peak No.	Elution Temp. (°C)	Compound	Chromato- graphic Peak No.	Elution Temp. (°C)	Compound
1	100-112	toluene (solvent)	34	258	methylpyrene isomer
2	109	trimethylbenzene isomer	35	260	C ₁₇ H ₁₂ isomer ⁵ (tent.)
3	110.5	trimethylbenzene isomer	36	263	unknown
4	112	C ₃ H ₇ benzene isomer	37	264	methylpyrene isomer
5	113	C ₄ H ₉ benzene isomer	38	265	unknown
6	116	C ₄ H ₉ and C ₄ H ₇ benzene isomers	39	265	terphenyl isomer (tent.) + tri phenyl phosphate (bkg.)
7	120	C ₄ H ₉ benzene isomer (tent.)	40	265	terphenyl isomer (tent.)
8	122	C ₄ H ₇ benzene isomer	41	265	C ₁₈ H ₁₀ isomer ⁴
9	127	naphthalene (tent.)	42	265	C ₁₈ H ₁₄ isomer ⁶
10	128	C ₅ H ₉ benzene isomer	43	265	C ₁₈ H ₁₀ isomer ⁴
11	136-139	mixture of alkanes	44	265	C ₁₈ H ₁₂ isomer ⁷
12	141	phthalic anhydride	45	265	C ₁₈ H ₁₂ isomer ⁷
13	142	methylnaphthalene isomer	46	265	C ₁₈ H ₁₂ isomer ⁷
14	167	dibutylcresol isomer (bkg.)	47	265	benzanthrone
15	172	unknown	48	265	di-2-ethylhexylphthalate (bkg.)
16	173	dibutylcresol isomer (bkg.)	49	265	C ₁₉ H ₁₄ isomer ⁸ (tent.)
17	177	C ₂ alkyl biphenyl (tent.)	50	265	long-chain saturated hydrocarbon
18	187	Si compd. (bkg.)	51	265	C ₂₀ H ₁₂ isomer ⁹
19	191	4-hydroxy-3,5-dimethoxy- benzaldehyde	52	265	C ₂₀ H ₁₂ isomer ⁹
20	198.5	C ₂ alkyl fluorene isomer (tent.)	53	265	C ₂₀ H ₁₄ isomer ¹⁰
21	201	C ₁₅ H ₁₆ isomer ¹	54	265	C ₂₀ H ₁₂ isomer ⁹
22	206	unknown	55	265	long-chain saturated hydrocarbon
23	207	C ₁₄ H ₁₀ isomer ²	56	265	long-chain saturated hydrocarbon
24	208	phenothiazine (tent.)	57	265	C ₂₂ H ₁₂ isomer ¹¹
25	212.5	xanthene (tent.)	58	265	C ₂₂ H ₁₂ isomer ¹¹
26	220.5	naphthindenone isomer (tent.)	59	265	C ₂₂ H ₁₂ isomer ¹¹
27	222	methyl C ₁₄ H ₁₀ isomer	60	265	C ₂₂ H ₁₂ isomer ¹¹
28	234.5	Si compd. (bkg.)			
29	241	C ₁₆ H ₁₀ isomer ³ (not pyrene)			
30	244	C ₁₆ H ₁₀ isomer ³ (not pyrene)			
31	247	pyrene + pyrene-d ₁₀ (ext. std.)			
32	248.5	C ₁₈ H ₁₀ isomer ⁴			
33	251	unknown			

Notes:

- ¹C₁₅H₁₆ isomers include diphenylpropane isomers, ditolymethane isomers, and C₃ alkyl biphenyl isomers.
- ²C₁₄H₁₀ isomers include anthracene, phenanthrene, and biphenylacetylene.
- ³C₁₆H₁₀ isomers include pyrene, fluoranthene, and diphenyldiacetylene.
- ⁴C₁₈H₁₀ isomers include 1,10-benzfluoranthene and 3,4-cyclopentapyrene.
- ⁵C₁₇H₁₂ isomers include methylpyrene isomers and benzofluorene isomers.
- ⁶C₁₈H₁₄ isomers include terphenyl isomers, styrylnaphthalene isomers, diphenylbenzene isomers, and dihydro-benzanthracene isomers.
- ⁷C₁₈H₁₂ isomers include chrysene, benzophenanthrene isomers, triphenylene, naphthacene, and benzanthracene isomers.
- ⁸C₁₉H₁₄ isomers include methyltriphenylene isomers, methylbenzanthracene isomers, methylchrysene isomers, and phenylfluorene.
- ⁹C₂₀H₁₂ isomers include perylenebenzpyrene isomers, and benzfluoranthene isomers.
- ¹⁰C₂₀H₁₄ isomers include binaphthyl isomers, anthracene benzyne adducts, 6,7-acechrysene, and triptycene.
- ¹¹C₂₂H₁₂ isomers include 1,12-benzperylene, anthranthrene, and 2,3-o-phenylenepylene.

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16. ABSTRACT Recently developed techniques for sampling and analysis of ambient air by GC/MS/COMP were applied to the Kanawha Valley, WV and Shenandoah Valley, VA to assess the levels of organic pollutants. Volatile and very volatile compounds were concentrated on Tenax GC and carbon sorbent cartridges, respectively, then thermally desorbed directly into the capillary column GC/MS/COMP system for analysis. Semivolatiles were collected on the electrostatic precipitator plates of a Massive Air Sampler, extracted, fractionated, and then analyzed by GC/MS/COMP. The Kanawha Valley contained a broad range of halogenated, ketone, aldehyde, ester, aromatic, aliphatic and polynuclear aromatic compounds. The Shenandoah Valley contained a narrower range of organics, but generally higher observed levels of the compounds quantitated.			
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