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Title/Desc:

TANK 241BY107 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
3/1994 & 10/1994

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 21. ECN **№ 625441**Proj.
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Page 2 of 2

1. ECN (use no. from pg. 1)

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15. Design Verification Required

☐ Yes
☒ No

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18. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 12. Enter the affected document number in Block 19.

SDD/DD	☐	Seismic/Stress Analysis	☐	Tank Calibration Manual	☐
Functional Design Criteria	☐	Stress/Design Report	☐	Health Physics Procedure	☐
Operating Specification	☐	Interface Control Drawing	☐	Spares Multiple Unit Listing	☐
Criticality Specification	☐	Calibration Procedure	☐	Test Procedures/Specification	☐
Conceptual Design Report	☐	Installation Procedure	☐	Component Index	☐
Equipment Spec.	☐	Maintenance Procedure	☐	ASME Coded Item	☐
Const. Spec.	☐	Engineering Procedure	☐	Human Factor Consideration	☐
Procurement Spec.	☐	Operating Instruction	☐	Computer Software	☐
Vendor Information	☐	Operating Procedure	☐	Electric Circuit Schedule	☐
OM Manual	☐	Operational Safety Requirement	☐	ICRS Procedure	☐
FSAR/SAR	☐	IEFD Drawing	☐	Process Control Manual/Plan	☐
Safety Equipment List	☐	Cell Arrangement Drawing	☐	Process Flow Chart	☐
Radiation Work Permit	☐	Essential Material Specification	☐	Purchase Requisition	☐
Environmental Impact Statement	☐	Fac. Proc. Samp. Schedule	☐	Tickler File	☐
Environmental Report	☐	Inspection Plan	☐		☐
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Characterization Results for Samples Collected in
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APPROVED FOR PUBLIC RELEASE

WHC Information Release Administration Specialist:

Kara Broz

9/26/95

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SUPPORTING DOCUMENT

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7. Abstract

Significant changes have been made to all of the original vapor characterization reports. This report documents specific headspace gas and vapor characterization results for all vapor sampling events to date. In addition, changes have been made to the original vapor reports to qualify the data based on quality assurance issues associated with the performing laboratories.

8.

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Tank 241-BY-107 Headspace Gas and Vapor Characterization Results for Samples Collected in March 1994 and October 1994

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Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
ISS	<i>in situ</i> sampling
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
ORNL	Oak Ridge National Laboratory
OGIST	Oregon Graduate Institute of Science and Technology
PNL	Pacific Northwest Laboratory
ppmv	parts per million by volume, 1 ppmv = 10 ⁻⁴ vol%
TNMOC	total nonmethane organic carbon
TST	triple sorbent trap
vol%	percent by volume, 1 vol% = 10,000 ppmv
VSS	vapor sampling system
WHC	Westinghouse Hanford Company

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Tank 241-BY-107 Headspace Gas and Vapor Characterization Results
for Samples Collected in March 1994 and October 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BY-107 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). This report primarily discusses results from the October 1994 sampling event, but also includes selected results of the March 1994 sampling event. The tank BY-107 headspace was sampled in March 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in October 1994 in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

1.2 Characterization Data Criteria

Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution describes parameters for data collection to ensure appropriate conclusions can be drawn from the data. Tank headspace characterization data were collected to help in the evaluation of 1) headspace flammability, and 2) identification and quantification of compounds of toxicological concern.

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank BY-107, specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995a).

Headspace characterization data are used by Westinghouse Hanford Company (WHC) Tank Waste Remediation Systems Industrial Hygiene as source term data in the industrial hygiene strategy to protect workers from tank fugitive emissions. Because selection of worker protective equipment must be based on industrial hygiene monitoring of the work place and not on source term data (29 CFR 1910.120), tank headspace characterization data can not be used for this purpose. Furthermore, because there are mechanisms by which headspace constituents can be either diluted or concentrated as they are released to the atmosphere, the headspace characterization data should not be considered to be representative of emissions at the point of emission.

These statements notwithstanding, the data quality objectives document specifies that the industrial hygiene group be advised if constituents with toxicological properties exceed 50 % of the appropriate consensus exposure standard (CES) for non-carcinogens, or 10 % of the appropriate CES for carcinogens. A CES is defined as the most stringent of known regulatory or recommended toxicological values for the workplace (Osborne et al. 1994).

1.3 Sampling Overview

Tank BY-107 was vapor sampled in March 1994 using the *in situ* sampling (ISS) method, and again in October 1994 using the more robust vapor sampling system (VSS) method. Unfortunately, the ISS event sorbent trap samples were radiologically contaminated, and were never analyzed (Huckaby et al. 1995). Furthermore, there are discrepancies between results from the ISS and VSS methods that are not understood (Huckaby 1994a), and until the ISS method has been validated and the discrepancies resolved, results from early ISS events should be considered suspect.

Nevertheless, a brief description of the ISS event and the total nonmethane organic carbon (TNMOC) measurement from the March 1994 ISS event are presented below, because this analysis was not performed on samples from the VSS event. All other results presented here are from the October 1994 VSS sampling event.

Samples collected are thought to have been representative of the tank headspace when the tank was sampled (Meacham et al. 1995), and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment has been made of how the tank BY-107 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in passively ventilated tanks, such as tank BY-107 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank BY-107 is the first tank in a 3-tank cascade with tanks BY-108 and BY-109. It is connected to tank BY-108 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. Tanks BY-108 and BY-109 are also connected by a similar line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank BY-108 or BY-109 may be transferred to tank BY-107 (except if the cascade lines are obstructed).

The cascade of tanks BY-107, BY-108, and BY-109 is passively ventilated, which means that the tanks are allowed to exhale air, waste gases, and vapors as the barometric pressure falls, and inhale ambient air as the barometric pressure rises. Each of these tanks has its own filtered breather riser. Barometric pressure typically rises and falls on a diurnal cycle, producing an average daily exchange of air equal to about 0.46 % of each tank headspace (Huckaby 1994b). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

2.1 March 1994 *In Situ* Sampling Event

Tank BY-107 was sampled using ISS methods on March 25, 1994 by WHC Sampling and Mobile Laboratories. This sampling was conducted to satisfy requirements of *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991). Samples were collected from a point approximately 6.7 m below the top of the flange on riser 12A, between 10:44 a.m. and 12:10 p.m. Though the sorbent traps were physically lowered down into the headspace to minimize loss of analytes through condensation, adsorption, or absorption by condensate, the SUMMA™ canister samples were collected using unheated transfer tubing.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1994) provides field sampling information for the tank BY-107 March 1994 ISS event. In addition to the TNMOC measurement results presented below, Sharma et al. (1995) and Rasmussen (1994) provide other sample analysis results.

2.2 October 1994 Vapor Sampling System Sampling Event

Headspace gas and vapor samples were collected from tank BY-107 using the VSS on October 26, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by the tank characterization plan (Carpenter 1994). The tank headspace temperature was determined to be 33.1 °C. Air from the tank BY-107 headspace was withdrawn via a 5.5 m-long heated sampling probe mounted in riser 5, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL). The 40 tank air samples and 2 ambient air control samples collected are listed in Table 2-1 by analytical laboratory. Table 2-1 also lists the 14 trip blanks and 2 field blanks that accompanied the samples.

A general description of vapor sampling and sample analysis methods is given by Huckaby et al. (1995). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC (1995b).

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL. Clauss et al. (1995) describe sample preparation and analyses.

Analyses of the VSS event inorganic vapor sorbent traps were performed within 21 days of sample collection, analyses of VSS event SUMMATM canisters for inorganic compounds were performed 83 days after sample collection (Ligotke 1995). Thus the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994) were fulfilled for analyses of only VSS sorbent traps. It should be noted that these inorganic compounds (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results may not have been affected even though the 60 day holding time requirements had been exceeded. PNL results were produced at PNL quality assurance impact level 2.

The relative standard deviations of the results, given in the last column in Table 3-1, indicate the precision of reported results is good. Relative standard deviations range from 0.6 % for ammonia, to 28 % for carbon dioxide results. The precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), and the relative standard deviations suggest there were no significant problems in the field or in the laboratories.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in tank BY-107 headspace was measured at 972 ppmv, and this concentration is among the highest observed to date in the waste tanks. Ammonia is thought to be a product of chemical and radiolytic waste degradation processes. It has been observed in virtually all of the waste tanks that have been sampled, at concentrations ranging from about 3 ppmv in C-108 (Lucke et al. 1995), to 1040 ppmv in tank BY-108 (McVeety et al. 1995). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 972 ppmv corresponds to less than 0.7 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The hydrogen concentration in tank BY-107 was determined to be 267 ppmv. In general, hydrogen is of concern as a fuel. The measured 267 ppmv of hydrogen in tank BY-107, however, represents only about 0.7 % of the LFL for hydrogen in air, and is not a flammability concern at this level.

The nitrous oxide concentration in tank BY-107 was measured to be 621 ppmv. This is a higher than typical concentration for the passively ventilated tanks that have been sampled, but concentrations have been as high as 878 ppmv in tank U-103 (Ligotke et al. 1995). Under proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank BY-107 headspace.

¹ SUMMA is a trademark of Molectrics, Inc., Cleveland, Ohio.

3.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 94 ppmv, is about one-fourth of the normal ambient air concentration of about 400 ppmv. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial liquid, and condensate) in the tank. The 94 ppmv carbon dioxide concentration measured in tank BY-107 is typical of other tanks sampled to date.

Carbon monoxide in the tank BY-107 headspace was measured to be < 20 ppmv. Its concentration in ambient air typically ranges from 0.05 to 0.15 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common, and have been measured to be as high as [26.7 ppmv] in tank C-103² (Huckaby and Story 1994). Elevated carbon monoxide concentrations are thought to be due to the decomposition of organic waste in the tanks.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BY-107 headspace were determined to be 0.13 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-107. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank BY-107 headspace.

The water vapor concentration of tank BY-107 was determined to be about 13.0 mg/L, at the tank headspace temperature of 33.1 °C and pressure of 981 mbar (735.7 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 18.31 mbar (13.7 torr), to a dew point of 16.1 °C, and to a relative humidity of 36 %.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium ions produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Analysis of the silica gel indicated the total activity of the headspace to be below 50 pCi/L (WHC 1995b).

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor and carbon dioxide, the most abundant waste constituents in the tank BY-107 headspace are ammonia, hydrogen, and nitrous oxide. These have been detected in most tank

² The carbon monoxide measurement in tank C-103 was made by Oregon Graduate Institute of Science and Technology, and placed in brackets to emphasize it should be considered secondary data.

headspaces sampled to date, and usually are the dominate waste species. In tank BY-107 these are each higher than typical for the passively ventilated tanks that have been sampled.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are very good. Relative standard deviations range from < 1 % for ammonia to 28 % for carbon dioxide. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), the small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

As discussed briefly in Section 1.4, it is possible that gases and vapors generated by the waste in tanks BY-108 and BY-109 could be transferred to tank BY-107 via the cascade lines. If significant exchange of selected inorganic gases and vapors were taking place between adjacent tanks, either their headspace compositions would be very similar (if the exchange is mutual), or all constituents detected in one tank would be at or equal or higher concentrations in the other tank (if air tends to flow consistently from one to the other). Consideration of data in Table 3-2 indicates that the headspace compositions of tanks BY-107 and BY-108 are quite similar, but with generally lower concentrations being found in tank BY-107. The data are consistent with the premise that the cascade line between them plays a significant role in their ventilation, but does not prove this occurs.

4.0 ORGANIC VAPORS

Organic vapors in the tank BY-107 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both laboratories used gas chromatographs (GCS) equipped with mass spectrometer (MS) detectors to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994) and Clauss et al. (1995). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method (EPA 1988) was also performed by Oregon Graduate Institute of Science and Technology (OGIST) on samples collected in March 1994 by the ISS method (Rasmussen 1994).

PNL SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-107. These results were produced at PNL quality assurance impact level 2. However, PNL analyses of organic vapors in SUMMA™ samples were not completed until 70 days after sample collection (Ligothe 1995), and this exceeded the administratively chosen 60-day holding time (Keller 1994). No holding time study has been performed to determine the stability of organic vapors in SUMMA™ canisters in the chemical matrix of tank air samples.

ORNL analyses of TST samples from this and other waste tanks generally agree with, support, and augment the SUMMA™ sample results. However, because certain WHC quality assurance requirements were not satisfied by ORNL, the quality assurance assessment of ORNL by Hendrickson (1995) should be reviewed before results unique to the TST samples are used for decision making.

All TSTs prepared by ORNL had 3 surrogate compounds added to evaluate sample matrix effects, potential handling, storage, and shipment problems, and analytical instrumentation performance (Jenkins et al. 1995). ORNL evaluated the surrogate recoveries using a statistical approach similar to that prescribed by *SW 846 Method 8260A Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS) Capillary Column Technique* (EPA 1992). Using this approach, ORNL reported that all surrogates had standard deviation values outside the 95 % confidence interval for variance, suggesting that a bias may have been introduced in the measurement of analyte quantities (Jenkins 1995a).

4.1 Positively Identified Organic Analytes

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained by analysis of standards. The concentration of an analyte in the sample is said to be quantitatively measured if the response of the GC/MS has been established at several known concentrations of that analyte (i.e., the GC/MS has been calibrated for that analyte), and the MS response to the analyte in the sample is between the lowest and highest responses to the known concentrations (i.e., the analyte is within the calibration range).

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list included 39 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of vapor data on tank C-103.

Listed in Table 4-1 are 13 organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL, and the result of analyses for methane. PNL performed analyses according to the EPA task order 14 (TO-14) methodology, but expanded the number of target analytes from 40 to 54 to include waste tank analytes of particular interest (EPA 1988, Clauss et al. 1995). Methane was analyzed with the inorganic gases, because it can not be analyzed using the TO-14 methodology. Of the original 40 TO-14 analytes, 37 were determined to be below the 0.002 ppmv quantitation limit of the analyses, and 4 of the 14 additional target analytes (ethanenitrile, pyridine, n-butanenitrile, and propanenitrile) were below the 0.005 ppmv method quantitation limit. Averages reported are from analyses of 3 SUMMA™ canister samples.

ORNL positively identified 24 of 27 target analytes selected by WHC. Three target analytes, 1,1-dichloroethene, tributyl phosphate, and dibutyl butylphosphonate, were below detection limits. Despite calibration of the instrument over about a 20-fold concentration range, the measured concentration of 12 of the 24 positively identified compounds was outside of the instrument calibration range in at least 1 of the 3 TST samples. Also, sample analyses were performed after the ORNL practical holding times of 3 analytes had been exceeded. Table 4-2 lists 11 quantitated compounds and their 3-TST average concentrations, Table 4-3 lists 10 positively identified but not quantitated compounds, and Table 4-3 lists the 3 compounds for which ORNL practical holding times had been exceeded. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so no compound appears in more than 1 of these tables. Data in Tables 4-3 and 4-4 may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

Based on a practical holding time study performed by ORNL the reported concentrations of butanal, 1-butanol, and 2-pentanone may have been affected by the 36 day period between sample collection and analysis (Jenkins 1995b). The concentration of these 3 analytes are reported in Table 4-4. The practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. Jenkins et al. (1995) describe the ORNL practical holding time study, and report practical holding times for butanal, 1-butanol, and 2-pentanone to be 1, 17, and 34 days respectively. It should be noted, however, that at the time of analysis the contractual holding time for the TST samples was 60 days.

Table 4-5 lists the 10 target analytes were common to both the ORNL and PNL analyses, and their reported average concentrations. Comparison of the results from the 2 laboratories indicates the following:

- 1) An acceptable agreement for the nonpolar analytes (i.e., n-hexane, benzene, n-heptane, toluene, and n-decane) and acetone; and
- 2) a significant disagreement regarding the existence of nitriles. Specifically, TST analyses indicate ethanenitrile at 2.2 ppmv, propanenitrile at 0.047 ppmv, n-butanenitrile at 0.12 ppmv, and n-pentanenitrile at 0.028 ppmv, while SUMMA™ analyses indicate each of these to be below their quantitation limits 0.005 ppmv.

That the nitriles observed in TST samples were not detected in SUMMA™ canister samples indicates there may have been a problem with recovery of nitriles from SUMMA™ canisters, or that they are lost in the sample conditioning steps. While it is also possible that TST samples were contaminated with the nitriles, it appears more likely that the nitriles were present in the tank headspace.

The most abundant analytes in Tables 4-1 through 4-4 are 1-butanol, propanone, ethanenitrile, 1-propanol, and 2-butanone. Each of these was measured to be above 1 ppmv. At the reported concentrations, these analytes do not individually or cumulatively represent a flammability hazard.

4.2 Tentatively Identified Organic Analytes

In addition to the target analytes, the ORNL and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and may also determine its molecular weight. The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Using this method, many analytes can be tentatively identified with reasonable confidence without having to inject each into the GC/MS to determine their GC retention times or specific MS patterns.

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and SUMMA™ samples. Analyses of the samples are designed to recover, separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (e.g., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (e.g., butanal) from SUMMA™ samples has been problematic.

The organic compounds tentatively identified in SUMMA™ canister samples by PNL are listed, with their estimated concentrations, in Table 4-6. Compounds are listed in Table 4-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table 4-7. Compounds are listed in Table 4-7 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

Because the list of tentatively identified organic compounds in TST samples is especially long (>200 compounds) and difficult to analyze, the list has been sorted alphanumerically by compound name in Table 4-8, and also in order of decreasing estimated concentrations in Table 4-9. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the location of the compound in Table 4-7.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 through 4-9 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables 4-6 through 4-9 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks or the assignment of the same identity to different peaks (e.g., Cmpd # 8 and 14 in Table 4-7). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

4.3 Total Nonmethane Organic Carbon

OGIST measured the TNMOC concentration in 3 SUMMA™ canister samples from the March 1994 ISS event using the EPA TO-12 method (Rasmussen 1994). Because OGIST did not have a WHC-approved quality assurance project plan in place during analyses, these results have been placed in brackets and should be considered secondary. The sample mean was [173 mg/m³], with a standard deviation of [6 mg/m³]. This is a relatively high TNMOC concentration for the waste tanks that have been sampled.

The sum of the ORNL target analyte concentrations, 55.2 mg/m³, and the ORNL estimated concentrations of tentatively identified analytes, 93.9 mg/m³, is 149.1 mg/m³. This value is in very good agreement (given method differences) with the EPA TO-12 value of 173 mg/m³.

4.4 Discussion of Organic Analytes

Some of the compounds listed in Tables 4-1 through 4-9 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane, n-tridecane, n-tetradecane, n-pentadecane) and methyl-substituted decahydronaphthalenes that were used as diluents for tributyl phosphate.

Most of the compounds in Tables 4-1 through 4-9 are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. For example, 1-butanol is known to be formed by the hydrolysis of tributyl phosphate, and it has been suggested that the alcohols, aldehydes, ketones, nitriles, alkenes, and short chain alkanes are all degradation products of the semivolatile NPHs.

In the semivolatile region of Tables 4-6 and 4-7, there are many branched alkanes. The abundance of these, as well as the decahydronaphthalenes, may indicate the origin of the tributyl phosphate diluent presently in tank BY-107.

Though their concentrations are not significant, many alcohols were tentatively identified by PNL and ORNL (Table 4-6, and 4-7). These have generally not been observed to be as numerous in other NPH-rich tank headspaces, which tend to be dominated by aldehydes, ketones, alkanes, and alkenes.

The tank BY-107 organic vapors may be indigenous to the waste in tank BY-107, but they may also be from tank BY-108. Table 3-2 lists for comparison both selected inorganic and organic headspace constituents. The data in Table 3-2 are consistent with the premise that a portion of the air introduced to tank BY-107 as it breathes with barometric pressure fluctuations, and due to other causes, comes from tank BY-108.

5.0 SUMMARY

The tank BY-107 headspace was sampled in March 1994 and October 1994 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the March 1994 event and essentially all results from the October 1994 event have been reported. It was determined that no headspace constituents exceeded the flammability notification limits, but that ammonia, measured to be 972 ppmv, exceeded the 150 ppmv industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Horn 1995).

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6.0 REFERENCES

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Table 2-1
Tank BY-107 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.05	Organic vapors	4 tank air samples
		0.25	Organic vapors	4 tank air samples
		0.50	Organic vapors	4 tank air samples
				+ 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
WHC 222-S Laboratory	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank BY-107 Inorganic Gas and Vapor Concentrations --
Analyses by Pacific Northwest Laboratory

Compound	CAS ¹ Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	972	6	0.6
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	94	26	28
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 20	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	267	36	14
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.13	0.03	23
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	621	36	6
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	18,700 (13.0 mg/L)	600 (0.4 mg/L)	3

1 CAS = Chemical Abstracts Service.

2 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 3-2
Comparison of Tank BY-107 and BY-108 Headspace Constituents¹

Tank:	BY-107	BY-108 ²
Date sampled, (mo/day/yr)	10/26/94	10/27/94
Headspace temperature, (°C)	33.1	25.7
Ammonia, (ppmv)	972	1040
Hydrogen, (ppmv)	267	399
Carbon dioxide, (ppmv)	94	224
Carbon monoxide, (ppmv)	< 20	<76
Nitric oxide, (ppmv)	0.13	≤ 0.03
Nitrogen dioxide, (ppmv)	≤ 0.02	≤ 0.02
Nitrous oxide, (ppmv)	621	641
Water vapor, (mg/m ³)	13.0	13.4
Water vapor, (% relative humidity)	36	56
Ethanenitrile (acetonitrile), (ppmv)	(2.2)	0.94
Propanone (acetone), (ppmv)	(3.9)	(8.2)
1-Butanol, (ppmv)	(7.9)	(58)
n-Dodecane, (ppmv)	0.21	0.80
n-Tridecane, (ppmv)	(0.26)	0.73
Total organic compounds ³ , (mg/m ³)	149.4	510

1 Inorganic gas or vapor results are from PNL; organic vapor results are from ORNL, with semiquantitative values in parentheses and quantitative values not in parentheses.

2 Data are from Huckaby and Bratzel 1995.

3 Total organic compound concentration was estimated from TST sample results.

Table 4-1
Tank BY-107 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Trichlorofluoromethane	75-69-4	0.030	0.002	7
2	Propanone (acetone)	67-64-1	6.5	0.7	10
3	1-Propanol	71-23-8	1.8	0.2	14
4	2-Butanone	78-93-3	1.1	0.03	3
5	n-Hexane	110-54-3	0.79	0.07	9
6	Benzene	71-43-2	0.0048	0.0003	6
7	4-Methyl-2-pentanone	108-10-1	0.028	0.003	12
8	Cyclohexane	110-82-7	0.078	0.048	62
9	n-Heptane	142-82-5	0.19	0.01	5
10	Tetrahydrofuran	109-99-9	0.56	0.01	1
11	Toluene	108-88-3	0.036	0.002	7
12	Cyclohexanone	108-94-1	0.0059	0.0022	38
13	n-Decane	124-18-5	0.033	0.003	9
14	Methane	74-82-8	< 20	--	--

1 CAS = Chemical Abstract Service.

2 Average of 3 samples.

3 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-2
Tank BY-107 Quantitatively Measured Organic Compound Average Concentrations --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	n-Butanenitrile	109-74-0	0.12	0.08	68
2	Toluene	108-88-3	0.067	0.007	11
3	n-Pentanenitrile	110-59-8	0.028	0.002	6
4	2-Hexanone	591-78-6	0.15	0.03	17
5	n-Octane	111-65-9	0.12	0.02	13
6	2-Heptanone	110-43-0	0.12	0.02	19
7	n-Nonane	111-84-2	0.066	0.005	8
8	2-Octanone	111-13-7	0.035	0.005	13
9	n-Decane	124-18-5	0.068	0.010	14
10	n-Undecane	1120-21-4	0.14	0.004	3
11	n-Dodecane	112-40-3	0.21	0.001	0.5

1 Results in this table are quantitative (as defined in Section 4.1).

2 CAS = Chemical Abstract Service.

3 Average of 3, 250 ml TST samples.

4 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-3
Tank BY-107 Positively Identified Organic Compound Average Concentrations
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	2.2	0.9	40
2	Propanone (acetone)	67-64-1	3.9	2.2	57
3	Dichloromethane	75-09-2	0.012	0.007	54
4	Propanenitrile	107-12-0	0.047	0.012	25
5	n-Hexane	110-54-3	0.94	0.12	13
6	Benzene	71-43-2	0.037	0.006	16
7	n-Heptane	142-82-5	0.35	0.12	34
8	n-Hexanenitrile	628-73-9	0.018	0.002	9
9	n-Heptanenitrile	629-08-3	0.013	0.002	18
10	n-Tridecane	629-50-5	0.26	0.01	4

1 Results in this table are not quantitative (as defined in Section 4.1) because measured values in at least 1 of the samples are outside instrument calibration limits.

2 CAS = Chemical Abstract Service.

3 Average of 3, 250 ml TST samples.

4 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

Table 4-4
Tank BY-107 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Butanal ⁵	123-72-8	0.13	0.20	153
2	1-Butanol ⁵	71-36-3	7.9	5.0	63
3	2-Pentanone ⁶	107-87-9	0.23	0.12	53

1 Practical holding times are defined and discussed in Section 4.1.

2 CAS = Chemical Abstract Service.

3 Average of 3, 250 ml TST samples.

4 RSD = relative standard deviation. Burnum (1995) specifies the RSD should be less than 25 %.

5 The concentration of this analyte was not quantitatively measured (as defined in Section 4.1), because the measured concentration was outside of the instrumental calibration limits.

6 The concentration of this analyte is quantitatively measured (as defined in Section 4.1).

Table 4-5
Tank BY-107 Comparison of Organic Compounds in TST and SUMMA™ Samples--
Analyses by Pacific Northwest Laboratory
and Oak Ridge National Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	PRD ⁴ (%)
Ethanenitrile (acetonitrile)	75-05-8	2.2	< 0.005	> 199
Propanone (acetone)	67-64-1	3.9	6.5	50
Propanenitrile	107-12-0	0.047	< 0.005	> 162
n-Hexane	110-54-3	0.94	0.79	17
Benzene	71-43-2	0.037	0.0048	154
n-Butanenitrile	109-74-0	0.12	< 0.005	> 184
n-Heptane	142-82-5	0.35	0.19	59
Toluene	108-88-3	0.067	0.036	60
n-Pentanenitrile	110-59-8	0.028	< 0.005	> 139
n-Decane	124-18-5	0.068	0.033	69

1 CAS = Chemical Abstract Service.

2 Average of 3, 250 ml TST samples.

3 Average of 3 samples from PNL.

4 PRD = percent relative difference. Keller (1994) requires the PRD to be less than 20 %.

Table 4-6
Tank BY-107 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propane	74-98-6	0.81	0.33
2	Propene	115-07-1	1.01	0.22
3	Cyclopropane	75-19-4	0.19	0.01
4	Isobutane	75-28-5	0.34	0.02
5	1-Butene	106-98-9	0.36	0.02
6	n-Butane	106-97-8	0.85	0.04
7	1-Propene, 2-methyl-	115-11-7	0.17	0.01
8	Isopropyl Alcohol	67-63-0	0.30	0.01
9	n-Pentane	109-66-0	0.55	0.00
10	2-Methylpentane	107-83-5	0.76	0.01
11	3-Methylpentane	96-14-0	0.15	0.00
12	2-Butanol	78-92-2	0.13	0.00
13	Methylcyclopentane	96-37-7	0.09	0.00
14	3-methyl-2-Butanone	563-80-4	0.12	0.00
15	1-Butanol	71-36-3	2.66	0.27
16	2-Pentanone	107-87-9	0.91	0.07
17	Hexane, 3-methyl-	589-34-4	0.53	0.01
18	2-Pentanol	6032-29-7	0.09	0.00
19	1-Heptene	592-76-7	0.08	0.00
20	C7 Alkene/Cycloalkane		0.07	0.00
21	2-Methyl-2-Pentanol	590-36-3	0.10	0.00
22	Methylcyclohexane	108-87-2	0.17	0.00
23	1-Pentanol	71-41-0	0.08	0.00
24	2-Methylheptane	592-27-8	0.30	0.01
25	2-Hexanone	591-78-6	0.31	0.01
26	n-Octane	111-65-9	0.29	0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Alkane		0.13	0.01
28	1,1,3-Trimethylcyclohexane	3073-66-3	0.11	0.01
29	3-Heptanone	106-35-4	0.22	0.01
30	2-Heptanone	110-43-0	0.23	0.00
31	n-Nonane	111-84-2	0.20	0.01
32	2-Heptanone, 6-methyl-	928-68-7	0.38	0.01
33	C3 substituted Cyclohexane		0.07	0.00
34	2-Octanone	111-13-7	0.10	0.00
35	C4 substituted Cyclohexane		0.09	0.00
36	C11 Alkane		0.22	0.01
37	C4 substituted Cyclohexane		0.16	0.03
38	C11 Alkane		0.07	0.00
39	n-Undecane	1120-21-4	0.71	0.02
40	Methyldecahydronaphthalene		0.11	0.02
41	Cyclohexane, pentyl-	4292-92-6	0.15	0.01
42	C12 Alkane		0.11	0.00
43	C12 Alkane		0.17	0.01
44	n-Dodecane	112-40-3	1.47	0.05
45	Decahydro-2,6-Dimethyl- naphthalene	1618-22-0	0.09	0.00
46	C13 Alkane		0.90	0.04
47	Decahydro-2,3-Dimethyl- naphthalene	1008-80-6	0.11	0.01
48	C7 substituted Cyclohexane		0.49	0.02
49	Unknown		0.16	0.01
50	Alkane		0.26	0.02
51	Alkane		0.17	0.01
52	Alkane		1.37	0.10
53	n-Tridecane	629-50-5	1.98	0.17

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
54	Alkene/Cycloalkane		0.08	0.01
55	Alkene/Cycloalkane		0.26	0.02
56	Alkane		0.30	0.02
57	Alkene/Cycloalkane		0.32	0.03
58	2-methyltridecane	1560-96-9	0.20	0.02
59	3-Methyltridecane	6418-41-3	0.11	0.01
60	C15 Alkane		1.20	0.10
61	n-Tetradecane	629-59-4	1.12	0.07
62	Alkene/Cycloalkane		0.13	0.01
63	Alkane		0.20	0.00
Sum of tentatively identified compounds:			25.57	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples, values listed are estimates.

Table 4-7
Tank BY-107 Tentatively Identified Organic Compounds in TST Samples
in the Order of Chromatographic Elution --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-propene, 2-methyl-	115-11-7	1.0	0.1
2	cyclopropane, 1,1-dimethyl-	1630-94-0	0.17	0.29
3	cyclobutane	287-23-0	0.15	0.26
4	butane, 2-methyl-	78-78-4	3.1	0.8
5	cyclopropane, ethyl-	1191-96-4	4.0	4.9
6	2-propanol	67-63-0	2.1	1.9
7	cyclopropane, ethyl-	1191-96-4	0.67	0.15
8	1-hexene	592-41-6	0.69	0.21
9	cyclopentane	287-92-3	0.43	0.38
10	pentane, 2-methyl-	107-83-5	6.9	1.6
11	1-propene, 2-fluoro-	1184-60-7	1.0	0.3
12	pentane, 3-methyl-	96-14-0	1.2	0.3
13	1-pentene, 2-methyl-	763-29-1	0.12	0.21
14	1-hexene	592-41-6	0.61	0.16
15	2-butanone	78-93-3	1.0	1.7
16	2-butanol	78-92-2	0.45	0.45
17	cyclopropane, propyl-	2415-72-7	0.53	0.28
18	cyclobutane, ethyl-	4806-61-5	0.19	0.33
19	1-pentene-2-methyl	763-29-1	0.29	0.50
20	furan, tetrahydro-	109-99-9	2.0	0.4
21	1,3-pentadiene, 2-methyl-	1118-58-7	0.14	0.24
22	hexane, 2-methyl-	591-76-4	0.61	0.20
23	alkanone		0.091	0.158
24	2-pentanol	6032-29-7	0.55	0.28
25	cyclohexane, methyl-	108-87-2	0.51	0.24
26	2-pentanol, 2-methyl-	590-36-3	0.078	0.135

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	2-pentanone, 4-methyl-	108-10-1	0.31	0.11
28	1-heptene, 6-methyl-	5026-76-6	0.054	0.094
29	hexane, 2,3-dimethyl-	584-94-1	0.70	0.67
30	furan, 2,5-dihydro-	1708-29-8	0.75	1.30
31	2(3H)-furanone, dihydro-3,5-dimethyl-	5145-01-7	0.17	0.30
32	3-pentanol, 2-methyl-	565-67-3	0.051	0.089
33	hexanal, 3-methyl-	19269-28-4	0.18	0.30
34	2-pentene, (E)-	646-04-8	0.24	0.41
35	3-hexanone	589-38-8	0.30	0.06
36	2-octanol	123-96-6	0.14	0.24
37	propane, 2,2'-oxybis-	108-20-3	0.15	0.25
38	methylamine, N-(1-methylbutylidene)-	22431-09-0	0.39	0.41
39	2-heptanol	543-49-7	0.092	0.159
40	tetrachloroethene	127-18-4	0.26	0.45
41	acetic acid, butyl ester	123-86-4	0.19	0.17
42	1,4-butanediol, dinitrate	3457-91-8	0.048	0.083
43	heptane, 2,6-dimethyl-	1072-05-5	0.29	0.09
44	cyclohexane, ethyl-	1678-91-7	0.24	0.09
45	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.67	0.46
46	1-hexene, 3,4-dimethyl-	16745-94-1	0.34	0.27
47	hexane, 3-methoxy-	54658-01-4	0.24	0.14
48	3-octanone	106-68-3	0.052	0.090
49	heptane, 2,3-dimethyl-	3074-71-3	0.040	0.070
50	octane, 2-methyl- and c2-benzene	3221-61-2	0.17	0.18
51	octane, 3-methyl- and c2-benzene	2216-33-3	0.17	0.29
52	benzene, ethyl and alkane	71-43-2	0.056	0.097
53	hexane, 2,2,3-trimethyl- and c2-benzene		0.54	0.54
54	4-heptanone	123-19-3	0.13	0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	unknown		0.042	0.073
56	3-heptanone	106-35-4	0.57	0.07
57	3-heptanol	589-82-2	0.31	0.22
58	2-heptanol	543-49-7	0.18	0.01
59	bicyclo[2.2.1]heptane	279-23-2	0.19	0.03
60	octane, 2,6-dimethyl-	2051-30-1	0.11	0.19
61	2-heptanone, 4-methyl-	6137-06-0	0.033	0.058
62	heptane, 4-(1-methylethyl)-	52896-87-4	0.028	0.048
63	3-pentanone, 2,4-dimethyl-	565-80-0	0.069	0.060
64	3-octanone	106-68-3	0.026	0.044
65	2-heptanone, 6-methyl-	928-68-7	1.0	0.2
66	nonane, 4-methyl-	17301-94-9	0.11	0.10
67	1,1,2,3-tetramethylcyclohexane	6783-92-2	0.27	0.04
68	nonane, 2-methyl-	871-83-0	0.042	0.072
69	2-octanol	123-96-6	0.27	0.07
70	3-butene-2-ol	598-32-3	0.67	0.37
71	decadienal		0.099	0.006
72	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	0.13	0.11
73	cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	0.037	0.064
74	phenol	108-95-2	0.029	0.050
75	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	0.20	0.17
76	3-hexene, 3-ethyl-2,5-dimethyl-	62338-08-3	0.093	0.160
77	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.092	0.102
78	cyclopentane, (1-methylbutyl)-	4737-43-3	0.079	0.137
79	nonane, 2,6-dimethyl-	17302-28-2	0.75	0.04
80	nonane, 3,7-dimethyl-	17302-32-8	0.028	0.049

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
81	nonane, 3,7-dimethyl-	17302-32-8	0.048	0.082
82	1-hexanol, 2-ethyl-	104-76-7	0.035	0.061
83	alkane		0.022	0.039
84	3-nonyne and others		0.024	0.041
85	cyclohexane, butyl-	1678-93-9	0.23	0.07
86	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.061	0.105
87	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.030	0.051
88	undecane, 5-methyl-	1632-70-8	0.047	0.081
89	cyclohexane, cyclopropyl	32669-86-6	0.061	0.053
90	1,1-dimethyl-2-propylcyclohexane		0.21	0.02
91	decane, 5-methyl-	13151-35-4	0.25	0.03
92	decane, 4-methyl-	2847-72-5	0.22	0.04
93	2-pentanone, 4-methyl-	108-10-1	0.23	0.39
94	octane, 2,3,3-trimethyl-	62016-30-2	0.47	0.42
95	naphthalene, decahydro-, trans-	493-02-7	0.18	0.17
96	decane, 3-methyl-	13151-34-3	0.43	0.22
97	2-furanacetaldehyde, .alpha.-propyl-	31681-26-2	0.14	0.12
98	4-nonanone and others		0.052	0.090
99	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.10	0.02
100	4-decene, 3-methyl-	62338-47-0	0.19	0.05
101	4-hepten-3-one, 5-ethyl-2,4-dimethyl	22319-29-5	0.16	0.15
102	5-undecene	4941-53-1	0.36	0.15
103	2-nonanone	821-55-6	0.29	0.05
104	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.11	0.03
105	5-undecene	4941-53-1	0.12	0.03
106	2-decene, 4-methyl-, (Z)-	74630-30-1	0.043	0.074
107	2-undecene, 2,5-dimethyl-	49622-16-4	0.030	0.053
108	undecane, 5-methyl-	1632-70-8	0.67	0.24

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
109	methyl-decahydronaphthalene		0.10	0.01
110	undecane, 2,8-dimethyl-	17301-25-6	0.40	0.49
111	naphthalene, decahydro-2-methyl	2958-76-1	0.35	0.32
112	undecane, 2,8-dimethyl-	17301-25-6	0.43	0.39
113	cyclopentane, 1-butyl-2-propyl-	62199-50-2	0.052	0.091
114	cyclohexane, pentyl-	4292-92-6	0.14	0.23
115	c4-heptadiene		0.29	0.50
116	cyclooctane, ethenyl-	61142-41-4	0.096	0.017
117	1-dodecene	112-41-4	0.026	0.044
118	3-undecene, 2-methyl-, (Z)-	74630-48-1	0.065	0.061
119	naphthalene, decahydro-2-methyl-	2958-76-1	0.99	0.91
120	6-methylundecane	17302-33-9	0.97	0.27
121	undecane, 4-methyl-	2980-69-0	0.52	0.11
122	undecane, 2-methyl-	7045-71-8	1.1	0.3
123	decane, 2,3,8-trimethyl-	62238-14-6	0.26	0.08
124	undecane, 3-methyl-	1002-43-3	0.60	0.13
125	2-undecene, 6-methyl-, (E)-	74630-61-8	0.060	0.105
126	decane, 2,6,7-trimethyl-	62108-25-2	0.18	0.17
127	decane, 2,3,6-trimethyl-	62238-12-4	0.18	0.03
128	cyclododecane	294-62-2	0.14	0.24
129	dimethyl-decahydronaphthalene		0.10	0.18
130	cyclotetradecane	295-17-0	0.27	0.23
131	naphthalene, decahydro-1,6-dimethyl	1750-51-2	0.10	0.18
132	cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.13	0.02
133	1,1'-bicyclohexyl	92-51-3	0.015	0.027
134	undecane, 2,4-dimethyl-	17312-80-0	0.048	0.042
135	undecane, 2,6-dimethyl-	17301-23-4	2.0	0.03
136	undecane, 3,7-dimethyl-	17301-29-0	0.20	0.02

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
137	decane, 2,3,5-trimethyl- and others		0.23	0.06
138	2-undecene, 7-methyl-, cis=trans		0.055	0.048
139	cyclopentane, 1-pentyl-2-propyl-	62199-51-3	0.023	0.040
140	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.80	0.01
141	undecane, 5-ethyl-	17453-94-0	0.098	0.013
142	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.10	0.04
143	dimethyl-decahydronaphthalene		0.076	0.068
144	cyclohexane, hexyl-	4292-75-5	0.67	0.06
145	undecane, 2,6-dimethyl-	17301-23-4	0.21	0.04
146	dodecane, 5-methyl-	17453-93-9	0.21	0.03
147	dodecane, 4-methyl-	6117-97-1	0.58	0.02
148	dodecane, 2-methyl-	1560-97-0	0.72	0.63
149	undecane, 2,10-dimethyl-	17301-27-8	0.34	0.59
150	dodecane, 4,6-dimethyl	61141-72-8	1.2	2.1
151	trimethyl-decahydronaphthalene		0.14	0.01
152	decane, 2,6,7-trimethyl-	62108-25-2	1.2	2.0
153	dodecane, 4,6-dimethyl	61141-72-8	1.1	2.0
154	trimethyl-decahydronaphthalene		0.12	0.11
155	cyclopentane, 1-butyl-2-ethyl-	72993-32-9	0.073	0.069
156	6-tridecene, 7-methyl-	24949-42-6	0.48	0.41
157	5-undecene, 7-methyl-, (Z)-	74630-62-9	0.037	0.064
158	3-tetradecene, (E)-	41446-68-8	0.24	0.41
159	c8-cyclopentane		0.13	0.11
160	c14-alkane		0.14	0.12
161	c14-alkane		0.23	0.20
162	tetradecane	629-59-4	0.84	0.55
163	c14-alkane		0.029	0.050
164	3,3,4,4-tetraethylhexane		0.027	0.047

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
165	undecane, 2,9-dimethyl-	17301-26-7	0.24	0.11
166	tridecane, 6-methyl	13287-21-3	0.38	0.66
167	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.19	0.16
168	tridecanenitrile	629-60-7	0.030	0.052
169	butane, 2-cyclohexyl-3-methyl-		0.055	0.095
170	tridecane, 3-methyl-	6418-41-3	0.079	0.137
171	1H-pyrrole, 1-pentyl and others		0.032	0.056
172	c5-octyne		0.046	0.079
173	tridecane, 6-methyl-	13287-21-3	0.59	0.10
174	c7-cyclohexane		1.1	0.1
175	tridecane, 4-methyl-	26730-12-1	0.91	0.02
176	tridecane, 2-methyl-	1560-96-9	1.3	0.04
177	undecane, 3,8-dimethyl-	17301-30-3	0.021	0.037
178	c14-alkene and others		0.068	0.118
179	dodecane, 3-methyl-	17312-57-1	0.63	0.59
180	undecane, 2,8-dimethyl-	17301-25-6	0.021	0.037
181	mixture		0.071	0.122
182	tridecane, 3-methyl-	6418-41-3	0.24	0.41
183	dodecane, 2,6,11-trimethyl-	31295-56-4	3.3	0.3
184	mixture		0.041	0.070
185	decane, 2-methyl-	6975-98-0	0.043	0.074
186	tetradecane	629-59-4	4.1	0.2
187	pentadecane	629-62-9	1.2	0.1
188	dodecane, 2,7,10-trimethyl-	74645-98-0	0.48	0.02
189	c14-alkene and others		0.40	0.01
190	c15-alkane		0.22	0.20
191	dodecane, 2,6,11-trimethyl-	31295-56-4	0.34	0.30
192	alkane		0.10	0.17

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
193	pentadecane	629-62-9	0.33	0.57
194	1-pentadecene	13360-61-7	0.11	0.19
195	tridecane, 3-ethyl-	13286-73-2	0.35	0.61
196	1-octanol, 2-butyl-	3913-02-8	0.11	0.18
197	tridecane, 5-propyl-	55045-11-9	1.2	1.4
198	dodecane, 3-methyl-	17312-57-1	0.15	0.26
199	tetradecane	629-59-4	0.11	0.19
200	nonane, 5-butyl-	17312-63-9	0.11	0.19
201	dodecane, 2-methyl-8-propyl-	55045-07-3	1.7	1.5
202	alkane		0.14	0.24
203	c16-alkane		0.11	0.18
204	hexadecane, 3-methyl-	6418-43-5	0.15	0.25
205	undecane, 5,7-dimethyl-	17312-83-3	0.11	0.19
206	7-hexadecene, (Z)-	35507-09-6	0.21	0.01
207	1h-indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	54832-83-6	0.20	0.01
208	pentadecane	629-62-9	2.5	0.2
209	1h-1,2,4-triazole, 1-ethyl-	16778-70-4	0.13	0.09
210	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-, cis-	54824-04-3	0.037	0.064
211	heptadecane, 2,6,10,14-tetramethyl-	18344-37-1	0.015	0.026
212	eicosane	112-95-8	0.11	0.19
213	dodecane, 2-methyl-8-propyl-	55045-07-3	0.14	0.12
214	tetradecane, 2,6,10-trimethyl-	14905-56-7	0.14	0.11
215	pentadecane, 8-hexyl-	13475-75-7	0.024	0.041
216	mixture		0.087	0.112
217	hexadecane, 2-methyl-	1560-92-5	0.044	0.039
218	alkane		0.029	0.050

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
219	dodecane, 5,8-diethyl	24251-86-3	0.025	0.044
220	hexadecane	544-76-3	0.48	0.05
221	pentadecane, 2,6,10-trimethyl- (non-pristan)	3892-00-0	0.063	0.055
222	ester of alkenoic acid		0.017	0.029
223	1-hexadecene	629-73-2	0.017	0.029
224	undecane, 3,6-dimethyl-	17301-28-9	0.034	0.058
225	hexadecanoic acid	57-10-3	0.020	0.035
226	alkene and others		0.018	0.032
227	tetradecanoic acid	544-63-8	0.27	0.23
228	1-hexadecanol, acetate	629-70-9	0.018	0.031
229	benzenamine, N-phenyl-	122-39-4	0.015	0.026
230	pentadecane	629-62-9	0.019	0.033
231	pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.019	0.033
232	tetradecanoic acid	544-63-8	0.11	0.19
233	benzenesulfonamide, n-butyl-	3622-84-2	0.38	0.04
234	9-octadecenoic acid (Z)-	112-80-1	0.030	0.026
235	9-octadecenoic acid (Z)-	112-80-1	0.016	0.028
236	14-pentadecenoic acid	17351-34-7	0.014	0.024
237	tetradecanoic acid	544-63-8	0.23	0.08
238	9-hexadecenoic acid	2091-29-4	0.52	0.14
239	hexadecanoic acid	57-10-3	1.1	0.3
240	eicosane	112-95-8	0.028	0.049
241	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.077	0.022
242	cyclohexadecane	295-65-8	0.024	0.041
243	1-hexadecanol	36653-82-4	0.039	0.067
Sum of tentatively identified compounds:			93.9	

1 CAS = Chemical Abstract Service.

2 Average of 3, 250 ml TST samples, values listed are estimates.

Table 4-8
Tank BY-107 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-propene, 2-methyl-	115-11-7	1.0	0.1
223	1-hexadecene	629-73-2	0.017	0.029
194	1-pentadecene	13360-61-7	0.11	0.19
117	1-dodecene	112-41-4	0.026	0.044
243	1-hexadecanol	36653-82-4	0.039	0.067
228	1-hexadecanol, acetate	629-70-9	0.018	0.031
19	1-pentene-2-methyl-	763-29-1	0.29	0.50
8	1-hexene	592-41-6	0.69	0.21
82	1-hexanol, 2-ethyl-	104-76-7	0.035	0.061
28	1-heptene, 6-methyl-	5026-76-6	0.054	0.094
11	1-propene, 2-fluoro-	1184-60-7	1.0	0.3
46	1-hexene, 3,4-dimethyl-	16745-94-1	0.34	0.27
13	1-pentene, 2-methyl-	763-29-1	0.12	0.21
14	1-hexene	592-41-6	0.61	0.16
196	1-octanol, 2-butyl-	3913-02-8	0.11	0.18
90	1,1-dimethyl-2-propylcyclohexane		0.21	0.02
133	1,1'-bicyclohexyl	92-51-3	0.015	0.027
21	1,3-pentadiene, 2-methyl-	1118-58-7	0.14	0.24
42	1,4-butanediol, dinitrate	3457-91-8	0.048	0.083
67	1,1,2,3-tetramethylcyclohexane	6783-92-2	0.27	0.04
236	14-pentadecenoic acid	17351-34-7	0.014	0.024
207	1h-indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	54832-83-6	0.20	0.01
209	1h-1,2,4-triazole, 1-ethyl-	16778-70-4	0.13	0.09
171	1H-pyrrole, 1-pentyl and others		0.032	0.056

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
24	2-pentanol	6032-29-7	0.55	0.28
26	2-pentanol, 2-methyl-	590-36-3	0.078	0.135
27	2-pentanone, 4-methyl-	108-10-1	0.31	0.11
15	2-butanone	78-93-3	1.0	1.7
16	2-butanol	78-92-2	0.45	0.45
6	2-propanol	67-63-0	2.1	1.9
125	2-undecene, 6-methyl-, (E)-	74630-61-8	0.060	0.105
58	2-heptanol	543-49-7	0.18	0.01
138	2-undecene, 7-methyl-, cis=trans		0.055	0.048
34	2-pentene, (E)-	646-04-8	0.24	0.41
61	2-heptanone, 4-methyl-	6137-06-0	0.033	0.058
36	2-octanol	123-96-6	0.14	0.24
65	2-heptanone, 6-methyl-	928-68-7	1.0	0.2
107	2-undecene, 2,5-dimethyl-	49622-16-4	0.030	0.053
39	2-heptanol	543-49-7	0.092	0.159
106	2-decene, 4-methyl-, (Z)-	74630-30-1	0.043	0.074
103	2-nonanone	821-55-6	0.29	0.05
97	2-furanacetaldehyde, .alpha.-propyl-	31681-26-2	0.14	0.12
93	2-pentanone, 4-methyl-	108-10-1	0.23	0.39
69	2-octanol	123-96-6	0.27	0.07
31	2(3H)-furanone, dihydro-3,5-dimethyl-	5145-01-7	0.17	0.30
35	3-hexanone	589-38-8	0.30	0.06
32	3-pentanol, 2-methyl-	565-67-3	0.051	0.089
48	3-octanone	106-68-3	0.052	0.090
70	3-butene-2-ol	598-32-3	0.67	0.37
76	3-hexene, 3-ethyl-2,5-dimethyl-	62338-08-3	0.093	0.160
118	3-undecene, 2-methyl-, (Z)-	74630-48-1	0.065	0.061
84	3-nonyne and others		0.024	0.041

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
158	3-tetradecene, (E)-	41446-68-8	0.24	0.41
64	3-octanone	106-68-3	0.026	0.044
63	3-pentanone, 2,4-dimethyl-	565-80-0	0.069	0.060
56	3-heptanone	106-35-4	0.57	0.07
57	3-heptanol	589-82-2	0.31	0.22
164	3,3,4,4-tetraethylhexane		0.027	0.047
100	4-decene, 3-methyl-	62338-47-0	0.19	0.05
54	4-heptanone	123-19-3	0.13	0.01
98	4-nonanone and others		0.052	0.090
101	4-hepten-3-one, 5-ethyl-2,4-dimethyl-	22319-29-5	0.16	0.15
102	5-undecene	4941-53-1	0.36	0.15
157	5-undecene, 7-methyl-, (Z)-	74630-62-9	0.037	0.064
105	5-undecene	4941-53-1	0.12	0.03
156	6-tridecene, 7-methyl-	24949-42-6	0.48	0.41
120	6-methylundecane	17302-33-9	0.97	0.27
206	7-hexadecene, (Z)-	35507-09-6	0.21	0.01
234	9-octadecenoic acid (Z)-	112-80-1	0.030	0.026
238	9-hexadecenoic acid	2091-29-4	0.52	0.14
235	9-octadecenoic acid (Z)-	112-80-1	0.016	0.028
41	acetic acid, butyl ester	123-86-4	0.19	0.17
83	alkane		0.022	0.039
192	alkane		0.10	0.17
202	alkane		0.14	0.24
218	alkane		0.029	0.050
23	alkanone		0.091	0.158
226	alkene and others		0.018	0.032
229	benzenamine, N-phenyl-	122-39-4	0.015	0.026
52	benzene, ethyl and alkane	71-43-2	0.056	0.097

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
233	benzenesulfonamide, n-butyl-	3622-84-2	0.38	0.04
59	bicyclo[2.2.1]heptane	279-23-2	0.19	0.03
4	butane, 2-methyl-	78-78-4	3.1	0.8
169	butane, 2-cyclohexyl-3-methyl-		0.055	0.095
189	c14-alkene and others		0.40	0.01
161	c14-alkane		0.23	0.20
163	c14-alkane		0.029	0.050
178	c14-alkene and others		0.068	0.118
160	c14-alkane		0.14	0.12
190	c15-alkane		0.22	0.20
203	c16-alkane		0.11	0.18
115	c4-heptadiene		0.29	0.50
172	c5-octyne		0.046	0.079
174	c7-cyclohexane		1.1	0.1
159	c8-cyclopentane		0.13	0.11
3	cyclobutane	287-23-0	0.15	0.26
18	cyclobutane, ethyl-	4806-61-5	0.19	0.33
128	cyclododecane	294-62-2	0.14	0.24
242	cyclohexadecane	295-65-8	0.024	0.041
25	cyclohexane, methyl-	108-87-2	0.51	0.24
44	cyclohexane, ethyl-	1678-91-7	0.24	0.09
45	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.67	0.46
85	cyclohexane, butyl-	1678-93-9	0.23	0.07
89	cyclohexane, cyclopropyl-	32669-86-6	0.061	0.053
104	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.11	0.03
114	cyclohexane, pentyl-	4292-92-6	0.14	0.23
132	cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.13	0.02
140	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.80	0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
144	cyclohexane, hexyl-	4292-75-5	0.67	0.06
167	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.19	0.16
210	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-, cis-	54824-04-3	0.037	0.064
116	cyclooctane, ethenyl-	61142-41-4	0.096	0.017
9	cyclopentane	287-92-3	0.43	0.38
72	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	0.13	0.11
73	cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	0.037	0.064
75	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	0.20	0.17
77	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.092	0.102
78	cyclopentane, (1-methylbutyl)-	4737-43-3	0.079	0.137
86	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.061	0.105
87	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.030	0.051
113	cyclopentane, 1-butyl-2-propyl-	62199-50-2	0.052	0.091
139	cyclopentane, 1-pentyl-2-propyl-	62199-51-3	0.023	0.040
155	cyclopentane, 1-butyl-2-ethyl-	72993-32-9	0.073	0.069
2	cyclopropane, 1,1-dimethyl	1630-94-0	0.17	0.29
5	cyclopropane, ethyl-	1191-96-4	4.0	4.9
7	cyclopropane, ethyl-	1191-96-4	0.67	0.15
17	cyclopropane, propyl-	2415-72-7	0.53	0.28
130	cyclotetradecane	295-17-0	0.27	0.23
71	decadienal		0.099	0.006
91	decane, 5-methyl-	13151-35-4	0.25	0.03
92	decane, 4-methyl-	2847-72-5	0.22	0.04
96	decane, 3-methyl-	13151-34-3	0.43	0.22
123	decane, 2,3,8-trimethyl-	62238-14-6	0.26	0.08
126	decane, 2,6,7-trimethyl-	62108-25-2	0.18	0.17

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
127	decane, 2,3,6-trimethyl-	62238-12-4	0.18	0.03
137	decane, 2,3,5-trimethyl- and others		0.23	0.06
152	decane, 2,6,7-trimethyl-	62108-25-2	1.2	2.0
185	decane, 2-methyl-	6975-98-0	0.043	0.074
129	dimethyl-decahydronaphthalene		0.10	0.18
143	dimethyl-decahydronaphthalene		0.076	0.068
146	dodecane, 5-methyl-	17453-93-9	0.21	0.03
147	dodecane, 4-methyl-	6117-97-1	0.58	0.02
148	dodecane, 2-methyl-	1560-97-0	0.72	0.63
150	dodecane, 4,6-dimethyl-	61141-72-8	1.2	2.1
153	dodecane, 4,6-dimethyl-	61141-72-8	1.1	2.0
179	dodecane, 3-methyl-	17312-57-1	0.63	0.59
183	dodecane, 2,6,11-trimethyl-	31295-56-4	3.3	0.3
188	dodecane, 2,7,10-trimethyl-	74645-98-0	0.48	0.02
191	dodecane, 2,6,11-trimethyl-	31295-56-4	0.34	0.30
198	dodecane, 3-methyl-	17312-57-1	0.15	0.26
201	dodecane, 2-methyl-8-propyl	55045-07-3	1.7	1.5
213	dodecane, 2-methyl-8-propyl-	55045-07-3	0.14	0.12
219	dodecane, 5,8-diethyl-	24251-86-3	0.025	0.044
212	eicosane	112-95-8	0.11	0.19
240	eicosane	112-95-8	0.028	0.049
222	ester of alkenoic acid		0.017	0.029
99	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.10	0.02
20	furan, tetrahydro-	109-99-9	2.0	0.4
30	furan, 2,5-dihydro-	1708-29-8	0.75	1.30
211	heptadecane, 2,6,10,14-tetramethyl-	18344-37-1	0.015	0.026
43	heptane, 2,6-dimethyl-	1072-05-5	0.29	0.09
49	heptane, 2,3-dimethyl-	3074-71-3	0.040	0.070

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
62	heptane, 4-(1-methylethyl)-	52896-87-4	0.028	0.048
204	hexadecane, 3-methyl-	6418-43-5	0.15	0.25
217	hexadecane, 2-methyl-	1560-92-5	0.044	0.039
220	hexadecane	544-76-3	0.48	0.05
225	hexadecanoic acid	57-10-3	0.020	0.035
239	hexadecanoic acid	57-10-3	1.1	0.3
241	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.077	0.022
33	hexanal, 3-methyl-	19269-28-4	0.18	0.30
22	hexane, 2-methyl-	591-76-4	0.61	0.20
29	hexane, 2,3-dimethyl-	584-94-1	0.70	0.67
47	hexane, 3-methoxy-	54658-01-4	0.24	0.14
53	hexane, 2,2,3-trimethyl and c2-benzene		0.54	0.54
109	methyl-decahydronaphthalene		0.10	0.01
38	methylamine, N-(1-methylbutylidene)-	22431-09-0	0.39	0.41
181	mixture		0.071	0.122
184	mixture		0.041	0.070
216	mixture		0.087	0.112
95	naphthalene, decahydro-, trans-	493-02-7	0.18	0.17
111	naphthalene, decahydro-2-methyl-	2958-76-1	0.35	0.32
119	naphthalene, decahydro-2-methyl-	2958-76-1	0.99	0.91
131	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.10	0.18
142	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.10	0.04
66	nonane, 4-methyl-	17301-94-9	0.11	0.10
68	nonane, 2-methyl-	871-83-0	0.042	0.072
79	nonane, 2,6-dimethyl-	17302-28-2	0.75	0.04
80	nonane, 3,7-dimethyl-	17302-32-8	0.028	0.049
81	nonane, 3,7-dimethyl-	17302-32-8	0.048	0.082
200	nonane, 5-butyl-	17312-63-9	0.11	0.19

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
50	octane, 2-methyl- and c2-benzene	3221-61-2	0.17	0.18
51	octane, 3-methyl- and c2-benzene	2216-33-3	0.17	0.29
60	octane, 2,6-dimethyl-	2051-30-1	0.11	0.19
94	octane, 2,3,3-trimethyl-	62016-30-2	0.47	0.42
187	pentadecane	629-62-9	1.2	0.1
193	pentadecane	629-62-9	0.33	0.57
208	pentadecane	629-62-9	2.5	0.2
215	pentadecane, 8-hexyl-	13475-75-7	0.024	0.041
221	pentadecane, 2,6,10-trimethyl- (non-pristan)	3892-00-0	0.063	0.055
230	pentadecane	629-62-9	0.019	0.033
231	pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.019	0.033
10	pentane, 2-methyl-	107-83-5	6.9	1.6
12	pentane, 3-methyl-	96-14-0	1.2	0.3
74	phenol	108-95-2	0.029	0.050
37	propane, 2,2'-oxybis-	108-20-3	0.15	0.25
40	tetrachloroethene	127-18-4	0.26	0.45
162	tetradecane	629-59-4	0.84	0.55
186	tetradecane	629-59-4	4.1	0.2
199	tetradecane	629-59-4	0.11	0.19
214	tetradecane, 2,6,10-trimethyl-	14905-56-7	0.14	0.11
227	tetradecanoic acid	544-63-8	0.27	0.23
232	tetradecanoic acid	544-63-8	0.11	0.19
237	tetradecanoic acid	544-63-8	0.23	0.08
166	tridecane, 6-methyl-	13287-21-3	0.38	0.66
170	tridecane, 3-methyl-	6418-41-3	0.079	0.137
173	tridecane, 6-methyl-	13287-21-3	0.59	0.10
175	tridecane, 4-methyl-	26730-12-1	0.91	0.02
176	tridecane, 2-methyl-	1560-96-9	1.3	0.04

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
182	tridecane, 3-methyl-	6418-41-3	0.24	0.41
195	tridecane, 3-ethyl-	13286-73-2	0.35	0.61
197	tridecane, 5-propyl-	55045-11-9	1.2	1.4
168	tridecanenitrile	629-60-7	0.030	0.052
151	trimethyl-decahydronaphthalene		0.14	0.01
154	trimethyl-decahydronaphthalene		0.12	0.11
88	undecane, 5-methyl-	1632-70-8	0.047	0.081
108	undecane, 5-methyl-	1632-70-8	0.67	0.24
110	undecane, 2,8-dimethyl-	17301-25-6	0.40	0.49
112	undecane, 2,8-dimethyl-	17301-25-6	0.43	0.39
121	undecane, 4-methyl-	2980-69-0	0.52	0.11
122	undecane, 2-methyl-	7045-71-8	1.1	0.3
124	undecane, 3-methyl-	1002-43-3	0.60	0.13
134	undecane, 2,4-dimethyl-	17312-80-0	0.048	0.042
135	undecane, 2,6-dimethyl-	17301-23-4	2.0	0.03
136	undecane, 3,7-dimethyl-	17301-29-0	0.20	0.02
141	undecane, 5-ethyl-	17453-94-0	0.098	0.013
145	undecane, 2,6-dimethyl-	17301-23-4	0.21	0.04
149	undecane, 2,10-dimethyl-	17301-27-8	0.34	0.59
165	undecane, 2,9-dimethyl-	17301-26-7	0.24	0.11
177	undecane, 3,8-dimethyl-	17301-30-3	0.021	0.037
180	undecane, 2,8-dimethyl-	17301-25-6	0.021	0.037
205	undecane, 5,7-dimethyl-	17312-83-3	0.11	0.19
224	undecane, 3,6-dimethyl-	17301-28-9	0.034	0.058
55	unknown		0.042	0.073
Sum of tentatively identified compounds:			93.9	

1 CAS = Chemical Abstract Service.

2 Average of 3, 250 ml TST samples, values listed are estimates.

Table 4-9
Tank BY-107 Tentatively Identified Organic Compounds in TST Samples
Sorted by Estimated Concentration --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
10	pentane, 2-methyl-	107-83-5	6.9	1.6
186	tetradecane	629-59-4	4.1	0.2
5	cyclopropane, ethyl-	1191-96-4	4.0	4.9
183	dodecane, 2,6,11-trimethyl-	31295-56-4	3.3	0.3
4	butane, 2-methyl-	78-78-4	3.1	0.8
208	pentadecane	629-62-9	2.5	0.2
6	2-propanol	67-63-0	2.1	1.9
20	furan, tetrahydro-	109-99-9	2.0	0.4
135	undecane, 2,6-dimethyl-	17301-23-4	2.0	0.03
201	dodecane, 2-methyl-8-propyl-	55045-07-3	1.7	1.5
176	tridecane, 2-methyl-	1560-96-9	1.3	0.04
12	pentane, 3-methyl-	96-14-0	1.2	0.3
197	tridecane, 5-propyl-	55045-11-9	1.2	1.4
187	pentadecane	629-62-9	1.2	0.1
150	dodecane, 4,6-dimethyl-	61141-72-8	1.2	2.1
152	decane, 2,6,7-trimethyl-	62108-25-2	1.2	2.0
174	c7-cyclohexane		1.1	0.1
153	dodecane, 4,6-dimethyl-	61141-72-8	1.1	2.0
239	hexadecanoic acid	57-10-3	1.1	0.3
122	undecane, 2-methyl-	7045-71-8	1.1	0.3
15	2-butanone	78-93-3	1.0	1.7
11	1-propene, 2-fluoro-	1184-60-7	1.0	0.3
1	1-propene, 2-methyl-	115-11-7	1.0	0.1
65	2-heptanone, 6-methyl-	928-68-7	1.0	0.2
119	naphthalene, decahydro-2-methyl-	2958-76-1	0.99	0.91
120	6-methylundecane	17302-33-9	0.97	0.27

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
175	tridecane, 4-methyl-	26730-12-1	0.91	0.02
162	tetradecane	629-59-4	0.84	0.55
140	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.80	0.01
30	furan, 2,5-dihydro	1708-29-8	0.75	1.30
79	nonane, 2,6-dimethyl-	17302-28-2	0.75	0.04
148	dodecane, 2-methyl-	1560-97-0	0.72	0.63
29	hexane, 2,3-dimethyl-	584-94-1	0.70	0.67
8	1-hexene	592-41-6	0.69	0.21
7	cyclopropane, ethyl-	1191-96-4	0.67	0.15
144	cyclohexane, hexyl-	4292-75-5	0.67	0.06
45	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.67	0.46
108	undecane, 5-methyl-	1632-70-8	0.67	0.24
70	3-butene-2-ol	598-32-3	0.67	0.37
179	dodecane, 3-methyl-	17312-57-1	0.63	0.59
22	hexane, 2-methyl-	591-76-4	0.61	0.20
14	1-hexene	592-41-6	0.61	0.16
124	undecane, 3-methyl-	1002-43-3	0.60	0.13
173	tridecane, 6-methyl-	13287-21-3	0.59	0.10
147	dodecane, 4-methyl-	6117-97-1	0.58	0.02
56	3-heptanone	106-35-4	0.57	0.07
24	2-pentanol	6032-29-7	0.55	0.28
53	hexane, 2,2,3-trimethyl- and c2-benzene		0.54	0.54
17	cyclopropane, propyl-	2415-72-7	0.53	0.28
121	undecane, 4-methyl-	2980-69-0	0.52	0.11
238	9-hexadecenoic acid	2091-29-4	0.52	0.14
25	cyclohexane, methyl-	108-87-2	0.51	0.24
188	dodecane, 2,7,10-trimethyl-	74645-98-0	0.48	0.02
156	6-tridecene, 7-methyl-	24949-42-6	0.48	0.41

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
220	hexadecane	544-76-3	0.48	0.05
94	octane, 2,3,3-trimethyl-	62016-30-2	0.47	0.42
16	2-butanol	78-92-2	0.45	0.45
96	decane, 3-methyl-	13151-34-3	0.43	0.22
112	undecane, 2,8-dimethyl-	17301-25-6	0.43	0.39
9	cyclopentane	287-92-3	0.43	0.38
189	c14-alkene and others		0.40	0.01
110	undecane, 2,8-dimethyl-	17301-25-6	0.40	0.49
38	methylamine, N-(1-methylbutylidene)-	22431-09-0	0.39	0.41
233	benzenesulfonamide, n-butyl-	3622-84-2	0.38	0.04
166	tridecane, 6-methyl-	13287-21-3	0.38	0.66
102	5-undecene	4941-53-1	0.36	0.15
195	tridecane, 3-ethyl-	13286-73-2	0.35	0.61
111	naphthalene, decahydro-2-methyl-	2958-76-1	0.35	0.32
46	1-hexene, 3,4-dimethyl-	16745-94-1	0.34	0.27
149	undecane, 2,10-dimethyl-	17301-27-8	0.34	0.59
191	dodecane, 2,6,11-trimethyl-	31295-56-4	0.34	0.30
193	pentadecane	629-62-9	0.33	0.57
57	3-heptanol	589-82-2	0.31	0.22
27	2-pentanone, 4-methyl-	108-10-1	0.31	0.11
35	3-hexanone	589-38-8	0.30	0.06
103	2-nonanone	821-55-6	0.29	0.05
19	1-pentene-2-methyl-	763-29-1	0.29	0.50
115	c4-heptadiene		0.29	0.50
43	heptane, 2,6-dimethyl-	1072-05-5	0.29	0.09
69	2-octanol	123-96-6	0.27	0.07
227	tetradecanoic acid	544-63-8	0.27	0.23
130	cyclotetradecane	295-17-0	0.27	0.23

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
123	decane, 2,3,8-trimethyl-	62238-14-6	0.26	0.08
40	tetrachloroethene	127-18-4	0.26	0.45
91	decane, 5-methyl-	13151-35-4	0.25	0.03
165	undecane, 2,9-dimethyl-	17301-26-7	0.24	0.11
44	cyclohexane, ethyl-	1678-91-7	0.24	0.09
47	hexane, 3-methoxy-	54658-01-4	0.24	0.14
34	2-pentene, (E)-	646-04-8	0.24	0.41
158	3-tetradecene, (E)-	41446-68-8	0.24	0.41
182	tridecane, 3-methyl-	6418-41-3	0.24	0.41
85	cyclohexane, butyl-	1678-93-9	0.23	0.07
93	2-pentanone, 4-methyl-	108-10-1	0.23	0.39
137	decane, 2,3,5-trimethyl- and others		0.23	0.06
237	tetradecanoic acid	544-63-8	0.23	0.08
161	c14-alkane		0.23	0.20
92	decane, 4-methyl-	2847-72-5	0.22	0.04
190	c15-alkane		0.22	0.20
206	7-hexadecene, (Z)-	35507-09-6	0.21	0.01
145	undecane, 2,6-dimethyl-	17301-23-4	0.21	0.04
146	dodecane, 5-methyl-	17453-93-9	0.21	0.03
136	undecane, 3,7-dimethyl-	17301-29-0	0.20	0.02
75	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	0.20	0.17
207	1h-indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	54832-83-6	0.20	0.01
100	4-decene, 3-methyl-	62338-47-0	0.19	0.05
41	acetic acid, butyl ester	123-86-4	0.19	0.17
59	bicyclo[2.2.1]heptane	279-23-2	0.19	0.03
167	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.19	0.16

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
18	cyclobutane, ethyl-	4806-61-5	0.19	0.33
126	decane, 2,6,7-trimethyl-	62108-25-2	0.18	0.17
95	naphthalene, decahydro-, trans-	493-02-7	0.18	0.17
127	decane, 2,3,6-trimethyl-	62238-12-4	0.18	0.03
58	2-heptanol	543-49-7	0.18	0.01
33	hexanal, 3-methyl-	19269-28-4	0.18	0.30
2	cyclopropane, 1,1-dimethyl-	1630-94-0	0.17	0.29
31	2(3H)-furanone, dihydro-3,5-dimethyl-	5145-01-7	0.17	0.30
50	octane, 2-methyl- and c2-benzene	3221-61-2	0.17	0.18
51	octane, 3-methyl- and c2-benzene	2216-33-3	0.17	0.29
101	4-hepten-3-one, 5-ethyl-2,4-dimethyl-	22319-29-5	0.16	0.15
3	cyclobutane	287-23-0	0.15	0.26
204	hexadecane, 3-methyl-	6418-43-5	0.15	0.25
37	propane, 2,2'-oxybis-	108-20-3	0.15	0.25
198	dodecane, 3-methyl-	17312-57-1	0.15	0.26
21	1,3-pentadiene, 2-methyl-	1118-58-7	0.14	0.24
114	cyclohexane, pentyl-	4292-92-6	0.14	0.23
202	alkane		0.14	0.24
151	trimethyl-decahydronaphthalene		0.14	0.01
128	cyclododecane	294-62-2	0.14	0.24
36	2-octanol	123-96-6	0.14	0.24
160	c14-alkane		0.14	0.12
97	2-furanacetaldehyde, .alpha.-propyl-	31681-26-2	0.14	0.12
214	tetradecane, 2,6,10-trimethyl-	14905-56-7	0.14	0.11
213	dodecane, 2-methyl-8-propyl-	55045-07-3	0.14	0.12
209	1h-1,2,4-triazole, 1-ethyl-	16778-70-4	0.13	0.09
132	cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.13	0.02

WHC-SD-WM-ER-421 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
72	Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	0.13	0.11
54	4-heptanone	123-19-3	0.13	0.01
159	c8-cyclopentane		0.13	0.11
105	5-undecene	4941-53-1	0.12	0.03
13	1-pentene, 2-methyl-	763-29-1	0.12	0.21
154	trimethyl-decahydronaphthalene		0.12	0.11
203	c16-alkane		0.11	0.18
60	octane, 2,6-dimethyl-	2051-30-1	0.11	0.19
66	nonane, 4-methyl-	17301-94-9	0.11	0.10
199	tetradecane	629-59-4	0.11	0.19
200	nonane, 5-butyl-	17312-63-9	0.11	0.19
104	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.11	0.03
205	undecane, 5,7-dimethyl-	17312-83-3	0.11	0.19
232	tetradecanoic acid	544-63-8	0.11	0.19
196	1-octanol, 2-butyl-	3913-02-8	0.11	0.18
194	1-pentadecene	13360-61-7	0.11	0.19
212	eicosane	112-95-8	0.11	0.19
192	alkane		0.10	0.17
142	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.10	0.04
129	dimethyl-decahydronaphthalene		0.10	0.18
131	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.10	0.18
109	methyl-decahydronaphthalene		0.10	0.01
71	decadienal		0.099	0.006
141	undecane, 5-ethyl-	17453-94-0	0.098	0.013
116	cyclooctane, ethenyl-	61142-41-4	0.096	0.017
76	3-hexene, 3-ethyl-2,5-dimethyl-	62338-08-3	0.093	0.160
39	2-heptanol	543-49-7	0.092	0.159
77	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.092	0.102

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
23	alkanone		0.091	0.158
216	mixture		0.087	0.112
170	tridecane, 3-methyl-	6418-41-3	0.079	0.137
78	cyclopentane, (1-methylbutyl)-	4737-43-3	0.079	0.137
26	2-pentanol, 2-methyl-	590-36-3	0.078	0.135
241	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.077	0.022
143	dimethyl-decahydronaphthalene		0.076	0.068
155	cyclopentane, 1-butyl-2-ethyl-	72993-32-9	0.073	0.069
181	mixture		0.071	0.122
63	3-pentanone, 2,4-dimethyl-	565-80-0	0.069	0.060
178	c14-alkene and others		0.068	0.118
118	3-undecene, 2-methyl-, (Z)-	74630-48-1	0.065	0.061
89	cyclohexane, cyclopropyl-	32669-86-6	0.061	0.053
86	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.061	0.105
125	2-undecene, 6-methyl-, (E)-	74630-61-8	0.060	0.105
52	benzene, ethyl and alkane	71-43-2	0.056	0.097
171	1H-pyrrole, 1-pentyl and others		0.032	0.056
221	pentadecane, 2,6,10-trimethyl- (non-pristan)	3892-00-0	0.063	0.055
169	butane, 2-cyclohexyl-3-methyl-		0.055	0.095
28	1-heptene, 6-methyl-	5026-76-6	0.054	0.094
98	4-nonanone and others		0.052	0.090
113	cyclopentane, 1-butyl-2-propyl-	62199-50-2	0.052	0.091
48	3-octanone	106-68-3	0.052	0.090
32	3-pentanol, 2-methyl-	565-67-3	0.051	0.089
138	2-undecene, 7-methyl-, cis=trans		0.055	0.048
81	nonane, 3,7-dimethyl-	17302-32-8	0.048	0.082
42	1,4-butanediol, dinitrate	3457-91-8	0.048	0.083
134	undecane, 2,4-dimethyl-	17312-80-0	0.048	0.042

WHC-SD-WM-ER-421 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
88	undecane, 5-methyl-	1632-70-8	0.047	0.081
172	c5-octyne		0.046	0.079
217	hexadecane, 2-methyl-	1560-92-5	0.044	0.039
185	decane, 2-methyl-	6975-98-0	0.043	0.074
106	2-decene, 4-methyl-, (Z)-	74630-30-1	0.043	0.074
55	unknown		0.042	0.073
68	nonane, 2-methyl-	871-83-0	0.042	0.072
184	mixture		0.041	0.070
67	1,1,2,3-tetramethylcyclohexane	6783-92-2	0.27	0.04
49	heptane, 2,3-dimethyl-	3074-71-3	0.040	0.070
243	1-hexadecanol	36653-82-4	0.039	0.067
157	5-undecene, 7-methyl-, (Z)-	74630-62-9	0.037	0.064
210	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-, cis-	54824-04-3	0.037	0.064
73	cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	0.037	0.064
82	1-hexanol, 2-ethyl	104-76-7	0.035	0.061
224	undecane, 3,6-dimethyl-	17301-28-9	0.034	0.058
61	2-heptanone, 4-methyl-	6137-06-0	0.033	0.058
87	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.030	0.051
107	2-undecene, 2,5-dimethyl-	49622-16-4	0.030	0.053
168	tridecanenitrile	629-60-7	0.030	0.052
234	9-octadecenoic acid (Z)-	112-80-1	0.030	0.026
163	c14-alkane		0.029	0.050
74	phenol	108-95-2	0.029	0.050
218	alkane		0.029	0.050
80	nonane, 3,7-dimethyl-	17302-32-8	0.028	0.049
240	eicosane	112-95-8	0.028	0.049
62	heptane, 4-(1-methylethyl)-	52896-87-4	0.028	0.048

WHC-SD-WM-ER-421 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
164	3,3,4,4-tetraethylhexane		0.027	0.047
117	1-dodecene	112-41-4	0.026	0.044
64	3-octanone	106-68-3	0.026	0.044
219	dodecane, 5,8-diethyl-	24251-86-3	0.025	0.044
84	3-nonyne and others		0.024	0.041
215	pentadecane, 8-hexyl-	13475-75-7	0.024	0.041
242	cyclohexadecane	295-65-8	0.024	0.041
139	cyclopentane, 1-pentyl-2-propyl-	62199-51-3	0.023	0.040
83	alkane		0.022	0.039
177	undecane, 3,8-dimethyl-	17301-30-3	0.021	0.037
180	undecane, 2,8-dimethyl-	17301-25-6	0.021	0.037
225	hexadecanoic acid	57-10-3	0.020	0.035
99	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.10	0.02
90	1,1-dimethyl-2-propylcyclohexane		0.21	0.02
230	pentadecane	629-62-9	0.019	0.033
231	pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.019	0.033
228	1-hexadecanol, acetate	629-70-9	0.018	0.031
226	alkene and others		0.018	0.032
222	ester of alkenoic acid		0.017	0.029
223	1-hexadecene	629-73-2	0.017	0.029
235	9-octadecenoic acid (Z)-	112-80-1	0.016	0.028
133	1,1'-bicyclohexyl	92-51-3	0.015	0.027
229	benzenamine, N-phenyl-	122-39-4	0.015	0.026
211	heptadecane, 2,6,10,14-tetramethyl-	18344-37-1	0.015	0.026
236	14-pentadecenoic acid	17351-34-7	0.014	0.024
Sum of tentatively identified compounds:			93.9	

1 CAS = Chemical Abstract Service.

2 Average of 3, 250 ml TST samples, values listed are estimates.

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