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TANK 241B103 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
2/1995

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ENGINEERING CHANGE NOTICE

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Page 2 of 2

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625435

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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	☐
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Environ.		Environ.	
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9/27/95

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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.

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Tank 241-B-103 Headspace Gas and Vapor Characterization Results for Samples Collected in February 1995

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Prepared for the U.S. Department of Energy
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Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
ORNL	Oak Ridge National Laboratory
PNL	Pacific Northwest Laboratory
ppmv	parts per million by volume, 1 ppmv = 10 ⁻⁴ vol%
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-B-103 Headspace Gas and Vapor Characterization Results
for Samples Collected in February 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank B-103 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). Tank B-103 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994). Results presented here represent the best available data on the headspace constituents of tank B-103.

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). However, current governing operating specifications for single shell Watchlist waste tanks, such as tank B-103, 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 B-103 headspace characterization data presented here are from a single 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 B-103 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 C-110 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank B-103 is the third tank in a 3-tank cascade with tanks B-101 and B-102. It is connected to tank B-102 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. Tanks B-101 and B-102 are connected by a similar line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank B-101 or tank B-102 may be transferred to tank B-103 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data is available for either tanks B-101 or B-102 to assess their potential effect on tank B-103.

The cascade of tanks B-101, B-102, and B-103 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 1994). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank B-103 using the vapor sampling system (VSS) on February 8, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-B-103 Tank Characterization Plan* (Carpenter 1995). The tank headspace temperature was determined to be 15.2 °C. Air from the B-103 headspace was withdrawn from a single elevation via a 7.9-m long heated sampling probe mounted in riser 2, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All tank air samples were collected between 12:03 p.m. and 4:25 p.m., with no anomalies noted.

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 provided by the laboratories.

A general description of vapor sampling and sample analysis methods is given by Huckaby and Babad (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^{TM,1} 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 and are given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were both prepared and analyzed by PNL (Ligotke et al. 1995a). PNL analyses of SUMMATM canisters and sorbent traps for inorganic compounds were performed 14 days after sample collection (Ligotke 1995), which was within the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994). PNL results were produced at PNL quality assurance impact level 2.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 8.8 ppmv, is among the lowest measured in the waste tanks to date. Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 1040 ppmv in BY-108 (McVeety et al. 1995). Given the LFL of ammonia in air is about 15 by volume (vol%), the measured 8.8 ppmv corresponds to about 0.006 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank B-103 was determined to be < 99 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, 99 ppmv of hydrogen would correspond to about 0.25 % of its LFL. At this level, hydrogen is not a flammability concern in tank B-103.

The nitrous oxide concentration in tank B-103 was measured to be 77.5 ppmv. Nitrous oxide has been detected in other passively ventilated waste tanks at average concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as 868 ppmv in tank U-103 (Ligotke et al. 1995b). Under the 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 B-103 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank B-103 headspace was measured to be < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide has not been measured at very high levels in any of the waste tanks, the highest level measured to date was [26.7 ppmv] in tank C-103² (Huckaby and Story 1994).

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

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.

The reported average carbon dioxide concentration in tank B-103 headspace SUMMA™ samples, 432 ppmv, is higher than it is in ambient air. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient in the waste tank headspaces. 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. Typical waste tank carbon dioxide concentrations are in the 20 to 200 ppmv range, however, elevated levels of carbon dioxide have been measured in tanks C-101 and C-107 (Huckaby and Bratzel 1995a, 1995b).

The apparent explanation of an elevated carbon dioxide concentration in tank B-103 is that the carbonate ion concentration in the liquid waste in the tank is high enough to produce an above-ambient carbon dioxide concentration in the air above it. This has been determined by Sederberg (1995) to explain the elevated carbon dioxide level in tank C-101.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank B-103 headspace were determined to be 0.46 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank B-103. 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 B-103 headspace.

The water vapor concentration of tank B-103 was determined to be about 9.9 mg/L, at the measured tank headspace temperature of 15.2 °C and pressure of 1000 mbar (750.2 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 13.2 mbar (9.9 torr), to a dew point of 11.1 °C, and to a relative humidity of 76 %.

Silica gel sorbent traps were used to sample for tritium. It is assumed that tritium 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. Radiochemical analysis of the silica gel trap indicated the total activity of the headspace to be less than 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 B-103 headspace are nitrous oxide and ammonia. These have been detected in most tank headspaces sampled to date, and along with hydrogen, are usually the dominate waste species.

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 less than 1 % for carbon dioxide to 13 % for nitrous oxide results. 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.

4.0 ORGANIC VAPORS

Organic vapors in the tank B-103 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both PNL and ORNL used a gas chromatograph (GC) equipped with a mass spectrometer (MS) to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Ligothke et al. (1995a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank B-103. PNL results were produced at PNL quality assurance impact level 2. All PNL analyses of organic vapors in SUMMA™ canisters were completed 20 days after sample collection, and satisfied the 60-day holding time. No holding time study has been performed to determine the stability of analytes in SUMMA™ canisters in the chemical matrix of the tank 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. 1995a). 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 within the 95 % confidence interval for variance, indicating that no bias was introduced in the measurement of analyte quantities (Jenkins 1995a).

4.1 Positively Identified Organic Compounds

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 when known compounds were analyzed. 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 from tank C-103.

Table 4-1 lists 14 organic compounds positively identified and quantitated in SUMMA™ samples. SUMMA™ organic analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Ligothke et al. 1995a). Only 1 of the 39 TO-14 target analytes and only 4 of the 14 additional target analytes were measured to be above the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

Jenkins et al. (1995) report the positive identification of 24 of 27 target analytes in TST samples. 1,1-Dichloroethene, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected in the TST samples. The average concentrations of 8 positively identified quantitated compounds, from the analysis of 3 TSTs, are given in Table 4-2. Table 4-3 lists 13 positively identified compounds for which the measured concentration in at least 1 of the TST samples was outside the instrument calibration range (i.e., not quantitated). The 3 other positively identified compounds are segregated in Table 4-4, because the ORNL practical holding time for these had been exceeded. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables.

The ORNL 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. As indicated in Table 4-4, of butanal, 1-butanol, and 2-pentanone exceeded their practical holding times, and may have been affected by the 38 day period between sample collection and analysis (Jenkins 1995b). Jenkins et al (1995b) describe the ORNL practical holding time study, and report practical holding times of butanal, 1-butanol, and 2-pentanone are 1, 17, and 34 days, respectively. It should be noted that the contractual holding time for the TST samples was 60 days.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMA™ samples. The data given in Table 4-5 indicate these methods agree that the 1,1-dichloroethene, dichloromethane, benzene, and n-decane concentrations are below the 0.005 ppmv detection limit of the SUMMA™ sample analysis. The methods are also in fair agreement on the concentration of n-heptane. However, ethanenitrile, propanenitrile, n-butanenitrile, toluene, and n-hexane were each measured in TST samples to be well above their SUMMA™ sample analysis detection limits. Conversely, SUMMA™ sample analyses indicate over twice as much propanone to be in the headspace as do the TST samples. Until the reasons for the discrepancies are determined at the laboratories, it is advisable to use the higher reported results.

The most abundant analytes in Tables 4-1 through 4-4 are propanone, tetrahydrofuran, 1-butanol, trichlorofluoromethane, 2-butanone, and n-tridecane, each of which was measured to be at or above 0.1 ppmv. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

4.2 Tentatively Identified Organic Compounds

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 list of tentatively identified compounds recovered from SUMMATM samples, with estimated concentrations, is given 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 they 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 rather long and finding any given compound may be difficult, 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 elution order 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. (1995) and Ligotke et al. (1995a), 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. Results in Tables 4-6 and 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 # 93, 98, and 112 in Table 4-7). In these instances, the estimated concentration of a compound appearing in different peaks is simply the sum of the individual peak estimates.

4.3 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-9 is to separate them into 2 categories: 1) Organic compounds added to tank B-103 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes the semivolatile branched and straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction processes. The semivolatile straight-chain alkanes (i.e., n-undecane, n-dodecane, n-tridecane, n-tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs).

The semivolatile alkane character of tank B-103 is different from that of the 241-BY and 241-C farm tanks, which are the best known at this time. Specifically, as is best shown in Table 4-8, there are numerous alkyl-substituted cyclohexanes, and the 14-carbon alkanes (i.e., n-tetradecane, methyltridecanes, and dimethyldodecanes) are prominent. Another distinction is that decahydronaphthalene and methyl-substituted decahydronaphthalenes, common in the 241-BY and certain 241-C farm tanks, are almost undetected in tank B-103, Cmpd # 75 in Table 4-7 being the only representative of this class of bicyclics. These differences in the character of the organic vapors are probably due to the different waste histories of these tanks.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 31 and 52 in Table 4-7) may also be in the category of waste additions. Small quantities of siloxanes may have been used as surfactants in various processes, and would have been introduced to the waste tank with other wastes. They may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-9 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, alkyl nitrates, volatile alkanes, and very low

volatility alkanes, all of which have been associated with the degradation of the NPHs. While both larger and smaller molecules are generated from the waste, the most abundant of these in the headspace are the smaller, short-chain volatile compounds.

The presence of the NPHs and their degradation products in tank B-103 is reason to expect trace amounts of tributyl phosphate to be present in the tank waste. Also, 1-butanol, known to be a product of the hydrolysis of tributyl phosphate, is one of the most abundant organic compounds detected in tank B-103 vapor samples. The low volatility of tributyl phosphate, and its tendency to adsorb on glass fiber filters during sampling, may preclude its measurement in the tank B-103 samples. Given these considerations, there is good reason to expect trace levels of tributyl phosphate do exist in the waste and in the headspace, despite the fact that it was not detected in any vapor samples.

The total organic vapor concentration of tank B-103 was estimated by Jenkins et al. to be about 9.8 mg/m³. This is the summation of concentrations of positively and tentatively identified compounds in 3 TST samples by GC/MS. A similar summation of the positively and tentatively identified organic compounds in SUMMA™ samples provides the estimate of 13.6 mg/m³.

The tank B-103 headspace has a moderate level of organic vapors compared to other waste tanks sampled to date. While having many of the same organic vapors as NPH-rich tanks, the character of the semivolatile alkanes in tank B-103 differs from that of the 241-BY and 241-C farm waste tanks.

5.0 SUMMARY

The tank B-103 headspace was sampled in February 1995 for gases and vapors to address flammability and industrial hygiene concerns. Collection and analysis of samples has been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

6.0 REFERENCES

- 29 CFR 1910.120, 1993, "Hazardous Waste Operations and Emergency Response", *Code of Federal Regulations*.
- Burnum, S. T., 1995, *Qualification of Reported WHC Vapor Program Data*, (letter 95-CHD-065 to president, Westinghouse Hanford Company, August 18), Department of Energy, Richland Operations Office, Richland, Washington.
- Carpenter, B. C., 1995, *Tank 241-B-103 Tank Characterization Plan*, WHC-SD-WM-TP-250, Westinghouse Hanford Company, Richland, Washington.
- Cashdollar, K. L., M. Hertzberg, I. A. Zlochower, C. E. Lucci, G. M. Green, and R. A. Thomas, 1992, *Laboratory Flammability Studies of Mixtures of Hydrogen, Nitrous Oxide, and Air*, WHC-SD-WM-ES-219 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Dougherty, L. F., 1995, *Single Shell Tank Interim Operational Safety Requirements*, WHC-SD-WM-OSR-005 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- EPA 1988, *Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air*, PB90-127374, U.S. Environmental Protection Agency, Washington, D.C.
- EPA 1992, *Test Methods for Evaluating Solid Waste*, SW-846 Rev. 1, U.S. Environmental Protection Agency, Washington, D.C.
- Hanlon, B. M., 1995, *Waste Tank Summary for Month Ending December 31, 1994*, WHC-EP-0182-81, Westinghouse Hanford Company, Richland, Washington.
- Hendrickson, R. W., 1995, *Tank Vapor Characterization Oak Ridge National Laboratories Quality Assurance Assessment*, TWRSQA-95-0012, Westinghouse Hanford Company, Richland, Washington.
- Homi, C. S., 1995, *Vapor Sampling and Analysis Plan*, WHC-SD-WM-TP-335 Rev. 0G, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., 1994, *Tank 241-C-103 Headspace Flammability*, WHC-EP-0734 Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., H. Babad, and D. R. Bratzel, 1995, *Headspace Gas and Vapor Characterization Summary for the 43 Vapor Program Suspect Tanks*, WHC-SD-WM-ER-514, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., and D. R. Bratzel, 1995a, *Tank 241-C-101 Headspace Gas and Vapor Characterization Results for Samples Collected in September 1994*, WHC-SD-WM-ER-458 Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., and D. R. Bratzel, 1995b, *Tank 241-C-107 Headspace Gas and Vapor Characterization Results for Samples Collected in September 1994*, WHC-SD-WM-ER-445 Rev. 1, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-WM-ER-438 REV. 1

- Huckaby, J. L., and M. S. Story, 1994, *Vapor Characterization of Tank 241-C-103*, WHC-EP-0780 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Jenkins, R. A., 1995a, *Untitled*, (Letter 090195 to D. Bratzel, September 1), Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Jenkins, R. A., 1995b, *Untitled*, (Letter 091495A to D. Bratzel, September 14), Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Jenkins, R. A., A. B. Dindal, C. Y. Ma, M. A. Palausky, J. T. Skeen, and C. K. Bayne, 1995a, *Analysis of Tank 241-B-103 Headspace Components*, ORNL-CASD-FR-241B103.95 Rev. 0, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Jenkins, R. A., A. B. Dindal, C. Y. Ma, M. A. Palausky, J. T. Skeen, and C. K. Bayne, 1995b, *Analysis of Tank 241-TY-104 Headspace Components*, ORNL-CASD-FR-241TY104.95 Rev. 1, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
- Keller, K.K., 1994, *Quality Assurance Project Plan for Tank Vapor Characterization*, WHC-SD-WM-QAPP-013 Rev.2, Westinghouse Hanford Company, Richland, Washington.
- Klinger, G. S., T. W. Clauss, M. W. Ligothke, K. H. Pool, R. B. Lucke, B. D. McVeety, O. P. Bredt, J. S. Young, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-TX-105: Results from Samples Collected Through the Vapor Sampling System on 12/20/94*, PNL-10594 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Ligothke, M. W. 1995, *PNL Vapor Project Analytical Holding Times*, (Letter to D.R. Bratzel, September 23, 1995), Pacific Northwest Laboratory, Richland, Washington.
- Ligothke, M. W., K. H. Pool, R. B. Lucke, B. D. McVeety, G. S. Klinger, T. W. Clauss, K. B. Olsen, O. P. Bredt, J. S. Fruchter, and S. C. Goheen, 1995a, *Vapor Space Characterization of Waste Tank 241-B-103: Results from Samples Collected on 2/8/95*, PNL-10704 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Ligothke, M. W., K. H. Pool, T. W. Clauss, B. D. McVeety, G. S. Klinger, K. B. Olsen, O. P. Bredt, J. S. Fruchter, and S. C. Goheen, 1995b, *Vapor Space Characterization of Waste Tank 241-U-103: Results from Samples Collected on 2/15/95*, PNL-10813 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Lucke, R. B., M. W. Ligothke, K. H. Pool, T. W. Clauss, A. K. Sharma, B. D. McVeety, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-C-108: Results from Samples Collected Through the Vapor Sampling System on 8/5/94*, PNL-10351 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Mahlum, D. D., J. Y. Young, and R. E. Weller, 1994, *Toxicologic Evaluation of Analytes from Tank 231-C-103*, PNL-10189, Pacific Northwest Laboratory, Richland, Washington.
- McVeety, B. D., T. W. Clauss, M. W. Ligothke, K. H. Pool, R. B. Lucke, G. S. Klinger, J. S. Young, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-BY-108: Results from Samples Collected on 10/27/94*, PNL-10495 UC-606, Pacific Northwest Laboratory, Richland, Washington.

WHC-SD-WM-ER-438 REV. 1

Meacham, J. E., H. Babad, R. J. Cash, G. T. Dukelow, S. J. Eberlein, D. W. Hamilton, G. D. Johnson, J. W. Osborne, M. A. Payne, D. J. Sherwood, D. A. Turner, and J. L. Huckaby, 1995, *Approach for Tank Safety Characterization of Hanford Site Waste*, WHC-EP-0843 Rev. 0, UC-2070, Westinghouse Hanford Company, Richland, Washington.

NFPA 1992, *Standard on Explosion Prevention Systems*, NFPA 69, National Fire Protection Association, Quincy, Massachusetts

Osborne, J. W., and J. L. Huckaby, 1994, *Program Plan for the Resolution of Tank Vapor Issues*, WHC-EP-0562 Rev. 1, Westinghouse Hanford Company, Richland, Washington.

Osborne, J. W., J. L. Huckaby, T. P. Rudolph, E. R. Hewitt, D. D. Mahlum, J. Y. Young, and C. M. Anderson, 1994, *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution*, WHC-SD-WM-DQO-002, Westinghouse Hanford Company, Richland, Washington.

WHC 1995a, *Operating Specifications for Watchlist Tanks*, OSD-T-151-00030, Rev. B-9, Westinghouse Hanford Company, Richland, Washington.

WHC 1995b, *Vapor and Gas Sampling of Single-Shell Tank 241-B-103 Using the Vapor Sampling System*, WHC-SD-WM-RPT-133, Westinghouse Hanford Company, Richland, Washington.

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Table 2-1
Tank B-103 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	0.2	Organic vapors	4 tank air samples
		1.0	Organic vapors	4 tank air samples
		4.0	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 blank
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blank
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Carbon dioxide, Carbon monoxide, Hydrogen, Methane, Nitrous oxide, Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank B-103 Inorganic Gas and Vapor Concentrations

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	8.8	0.8	9
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	432	0.6	0.1
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 99	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.46	0.06	13
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	77.5	1.6	2.1
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	13,200 (9.9 mg/L)	350 (0.3 mg/L)	2.7

1 CAS = Chemical Abstracts Service.

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

Table 4-1
Tank B-103 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	0.20	0.03	15
2	2-Butanone	78-93-3	0.14	0.01	4
3	Propanone (acetone)	67-64-1	0.28	0.05	19
4	n-Heptane	142-82-5	0.044	0.0004	1
5	Tetrahydrofuran	109-99-9	0.22	0.001	0.4
6	Methane	74-82-8	< 61	--	--
Sum of positively identified compounds:			3.28	mg/m ³	

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 B-103 Quantitatively Measured Organic Compounds in TST Samples –
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	0.072	0.014	20
2	Propanone (acetone)	67-64-1	0.13	0.012	9
3	n-Hexane	110-54-3	0.030	0.001	2
4	n-Heptane	142-82-5	0.034	0.002	6
5	Toluene	108-88-3	0.011	0.0003	3
6	n-Octane	111-65-9	0.0066	0.0010	15
7	n-Undecane	1120-21-4	0.013	0.001	10
8	n-Dodecane	112-40-3	0.037	0.004	11

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L samples.

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

Table 4-3
Tank B-103 Positively Identified Organic Compounds in TST Samples --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Dichloromethane (methylene chloride)	75-09-2	0.0014	0.0009	66
2	Propanenitrile	107-12-0	0.011	0.002	18
3	Benzene	71-43-2	0.004	0.0003	6
4	n-Butanenitrile	109-74-0	0.011	0.002	22
5	n-Pentanenitrile	110-59-8	0.0049	0.0006	13
6	2-Hexanone	591-78-6	0.0041	0.0006	15
7	n-Hexanenitrile	628-73-9	0.0037	0.0004	12
8	2-Heptanone	110-43-0	0.0039	0.0003	9
9	n-Nonane	111-84-2	0.0030	0.0007	23
10	n-Heptanenitrile	629-08-3	0.0032	0.0002	6
11	2-Octanone	111-13-7	0.0014	0.0001	7
12	n-Decane	124-18-5	0.0031	0.0004	12
13	n-Tridecane	629-50-5	0.12	0.02	17

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, 1-L samples.

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

Table 4-4
Tank B-103 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	0.092	0.020	21
2	1-Butanol ⁶	71-36-3	0.20	0.03	16
3	2-Pentanone ⁶	107-87-9	0.0082	0.0008	9

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L samples.

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

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

6 The concentration of this analyte was not quantitatively measured (as defined in Section 4.1), because its measured concentration in at least 1 TST sample was outside of the instrumental calibration limits.

Table 4-5
Tank B-103 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 (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.0023	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	0.0014	< 0.005	--
Propanone (acetone)	67-64-1	0.13	0.28	73
Ethanenitrile (acetonitrile)	75-05-8	0.072	< 0.005	> 174
Propanenitrile	107-12-0	0.011	< 0.005	> 75
n-Butanenitrile	109-74-0	0.011	< 0.005	> 75
Benzene	71-43-2	0.004	< 0.005	--
Toluene	108-88-3	0.011	< 0.005	> 75
n-Hexane	110-54-3	0.030	< 0.005	> 143
n-Heptane	142-82-5	0.034	0.044	26
n-Decane	124-18-5	0.0031	< 0.005	--

1 CAS = Chemical Abstract Service.

2 Average of 3 TST, 1-L samples by ORNL.

3 Average of 3 samples by PNL.

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

Table 4-6
Tank B-103 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
1	Propane	74-98-6	0.47	0.07
2	Cyclopropane	75-19-4	0.35	0.06
3	Ethanal (acetaldehyde)	75-07-0	0.22	0.05
4	n-Butane	106-97-8	0.82	0.12
5	2-Methyl-1-propene	115-11-7	0.17	0.02
6	Ethanol ⁴	64-17-5	0.12	--
7	Ethanenitrile ⁴ (acetonitrile)	75-05-8	0.12	--
8	n-Pentane	109-66-0	0.34	0.07
9	Methyl nitrate	598-58-3	0.17	0.11
10	2-Methyl-pentane	107-83-5	0.15	0.004
11	Butanal	123-72-8	0.29	0.01
12	Nitric acid, ethyl ester ⁴	625-58-1	0.30	--
13	Formic acid, 2-methylpropyl ester ⁵	542-55-2	0.30	< 0.17
14	1-Butanol	71-36-3	0.99	0.13
15	Nitric acid, propyl ester	627-13-4	0.69	0.01
16	Nitric acid, butyl ester	928-45-0	0.28	0.004
17	3-Heptanone ⁵	106-35-4	0.12	< 0.015
18	Unknown Alkyl Nitrate		0.36	0.01
19	n-Undecane	1120-21-4	0.16	0.01
20	n-Dodecane	112-40-3	0.70	0.03
21	2,6-Dimethyl-undecane	17301-23-4	0.15	0.004
22	Unknown Alkane		0.34	0.02
23	n-Tridecane	629-50-5	1.67	0.13
24	Unknown C15 Alkane		0.42	0.04
25	n-Tetradecane	629-59-4	0.95	0.10
26	Unknown C20 Alkane		0.15	0.01
Sum of tentatively identified compounds:			10.27	

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 sample, values listed are estimates.

3 When the analyte was detected in only 2 samples, the entry is the relative difference (i.e., their difference divided by 2).

4 Detected in only 1 sample.

5 Detected in only 2 samples.

Table 4-7
 Tank B-103 Tentatively Identified Organic Compounds in TST Samples
 in Order of Chromatographic Elution Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Cyclopropane	75-19-4	0.056	0.017
2	Isobutane	75-28-5	0.0055	0.0095
3	1-Propene, 2-methyl-	115-11-7	0.078	0.009
4	Butane	106-97-8	0.15	0.02
5	1-Propene, 2-methyl-	115-11-7	0.037	0.010
6	Ethanol	64-17-5	0.039	0.012
7	Butane, 2-methyl-	78-78-4	0.031	0.002
8	Trichlorofluoromethane	75-69-4	0.25	0.11
9	1-Pentene	109-67-1	0.0050	0.0087
10	Methyl nitrate	598-58-3	0.014	0.012
11	Pentane, 2-methyl-	107-83-5	0.039	0.001
12	1-Propanol	71-23-8	0.10	0.02
13	Pentane, 3-methyl-	96-14-0	0.0046	0.0080
14	3-Buten-2-one	78-94-4	0.022	0.002
15	2-Butanone	78-93-3	0.044	0.009
16	Nitric acid, ethyl ester	625-58-1	0.092	0.019
17	Furan, tetrahydro-	109-99-9	0.034	0.003
18	Formic acid, butyl ester	592-84-7	0.012	0.011
19	3-Heptene	592-78-9	0.026	0.007
20	2-Heptene	592-77-8	0.021	0.003
21	2-Heptene, (E)-	14686-13-6	0.021	0.019
22	Cyclopropane, butyl	930-57-4	0.021	0.001
23	Nitric acid, propyl ester	627-13-4	0.090	0.015
24	Propane, 2-methyl-2-nitro-	594-70-7	0.022	0.002
25	Heptane, 3-methyl-	589-81-1	0.048	0.001
26	trans-1-Butyl-2-methylcyclopropane	38851-70-6	0.0036	0.0063
27	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0067	0.0059

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	Hexanal	66-25-1	0.0058	0.0100
29	Furan, tetrahydro-2,4-dimethyl-, trans	39168-02-0	0.014	0.001
30	Tetrachloroethylene	127-18-4	0.036	0.001
31	Cyclotrisiloxane, hexamethyl	541-05-9	0.033	0.008
32	Nitric acid, butyl ester	928-45-0	0.13	0.01
33	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.0032	0.0056
34	Cyclopentanone, 2,2,5-trimethyl-	4573-09-5	0.0097	0.0086
35	Ethylbenzene	100-41-4	0.016	0.001
36	Pentane, 2,3-dimethyl-	565-59-3	0.033	0.002
37	p-Xylene	106-42-3	0.043	0.006
38	3-Heptanone	106-35-4	0.084	0.004
39	3-Heptanol	589-82-2	0.070	0.002
40	Benzene, 1,3-dimethyl-	108-38-3	0.015	0.001
41	Heptanal	111-71-7	0.018	0.005
42	1-Heptene	592-76-7	0.013	0.012
43	2,5-Pyrrolidinedione, 1-methyl-	1121-07-9	0.028	0.001
44	1,5-Pentanediol, dinitrate	3457-92-9	0.028	0.001
45	4-Heptanone, 3-methyl-	15726-15-5	0.020	0.001
46	2,2'-Bioxepane	74793-02-5	0.036	0.002
47	2-Pentene, 2,4-dimethyl-	625-65-0	0.037	0.002
48	2-Heptanone, 6-methyl-	928-68-7	0.11	0.01
49	5-Decene, (E)-	7433-56-9	0.015	0.014
50	1-Hexanol, 2-ethyl-	104-76-7	0.011	0.018
51	1-Heptanol	111-70-6	0.030	0.003
52	Cyclotetrasiloxane, octamethyl	556-67-2	0.11	0.04
53	.alpha.-Methylstyrene	98-83-9	0.0091	0.0079
54	3-Heptene, 4-propyl-	4485-13-6	0.0042	0.0073
55	Butanoic acid, butyl ester	109-21-7	0.033	0.004
56	Octanal	124-13-0	0.018	0.006

WHC-SD-WM-ER-438 REV. 1

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
57	1-Decene	872-05-9	0.016	0.003
58	Decane, 4-methyl-	2847-72-5	0.0096	0.0015
59	Nitric acid, hexyl ester	20633-11-8	0.014	0.002
60	1-Hexanol, 2-ethyl-	104-76-7	0.049	0.008
61	2-Pentene, 4,4-dimethyl-, (E) & others		0.013	0.001
62	Tridecane, 4-methyl-	26730-12-1	0.0067	0.0061
63	Nitric acid, pentyl ester	1002-16-0	0.12	0.04
64	5-Undecene, (Z)-	764-96-5	0.0099	0.0012
65	2-Heptanone, 6-methyl-	928-68-7	0.0097	0.0018
66	1-Octanol	111-87-5	0.0062	0.0055
67	3-t-Pentylcyclopentanone and others		0.011	0.003
68	Nonanenitrile	2243-27-8	0.021	0.003
69	Hexyl n-valerate	1117-59-5	0.017	0.001
70	2-Nonanone	821-55-6	0.0062	0.0054
71	Nonanal	124-19-6	0.025	0.005
72	Undecane, 2-methyl-	7045-71-8	0.013	0.001
73	Benzoic acid, 2-[(tri-methylsilyl)oxyl]-, trimethylsilyl ester	3789-85-3	0.021	0.019
74	n-Amylcyclohexane	4292-92-6	0.021	0.003
75	Naphthalene, decahydro-2-methyl-	2958-76-1	0.011	0.001
76	Undecane, 6-methyl-	17302-33-9	0.011	0.002
77	Undecane, 4-methyl-	2980-69-0	0.010	0.002
78	Decane, 3-methyl-	13151-34-3	0.018	0.002
79	Decane, 3,8-dimethyl-	17312-55-9	0.016	0.002
80	Nonanol	28473-21-4	0.0069	0.0120
81	Nonanenitrile	2243-27-8	0.023	0.003
82	Cyclohexane, 1-methyl-2-pentyl	54411-01-7	0.033	0.004
83	C6-cyclohexane		0.031	0.005
84	Undecane, 2,6-dimethyl-	17301-23-4	0.15	0.02

WHC-SD-WM-ER-438 REV. 1

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
85	Undecane, 2,4-dimethyl-	17312-80-0	0.030	0.005
86	1-Undecene	821-95-4	0.014	0.002
87	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.054	0.004
88	Cyclohexane, octyl	1795-15-9	0.10	0.01
89	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.012	0.010
90	Dodecane, 4-methyl-	6117-97-1	0.036	0.005
91	Undecane, 2,10-dimethyl-	17301-27-8	0.048	0.006
92	Cyclohexane, 1,1'-(1-methylethylidene)bis-	54934-90-6	0.023	0.001
93	Tridecane, 7-methyl-	26730-14-3	0.26	0.03
94	Cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.033	0.004
95	2(3H)-benzofuranone, 3a,4,5,6-tetrahydro-3a, 6,6-trimethyl	16778-26-0	0.021	0.005
96	3-Undecanone & undecanenitrile		0.0089	0.0079
97	Undecane, 4,8-dimethyl-	17301-33-6	0.012	0.003
98	Tridecane, 7-methyl-	26730-14-3	0.024	0.006
99	Tridecane, 6-methyl-	13287-21-3	0.12	0.02
100	Cyclohexane,(2-ethyl-1-methylbutylidene)-	74810-41-6	0.0086	0.0084
101	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.0039	0.0068
102	Cyclohexane, (1,2-dimethylbutyl)-		0.0055	0.0048
103	Dodecane, 2,5-dimethyl-	56292-65-0	0.031	0.006
104	Tridecane, 4-methyl-	26730-12-1	0.12	0.02
105	Tridecane, 2-methyl-	1560-96-9	0.075	0.012
106	Tetradecane, 4-methyl	25117-24-2	0.064	0.012
107	Dodecane, 4,6-dimethyl-	61141-72-8	0.43	0.06
108	3-Dodecanone	1534-27-6	0.020	0.020
109	Tetradecane	629-59-4	0.72	0.13
110	Tridecane, 4,8-dimethyl-	55030-62-1	0.096	0.010
111	Cyclohexane, 1,1,3- trimethyl-2-(3-methylpentyl)-	54965-05-8	0.091	0.017

WHC-SD-WM-ER-438 REV. 1

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
112	Tridecane, 7-methyl-	26730-14-3	0.0081	0.0071
113	Tetradecane, 4-methyl-	25117-24-2	0.021	0.004
114	Tetradecane, 3-methyl-	18435-22-8	0.029	0.002
115	6-Tridecanone	22026-12-6	0.069	0.013
116	5-Decanol	5205-34-5	0.025	0.007
117	3-Tridecanone	1534-26-5	0.061	0.013
118	Pentadecane	629-62-9	0.31	0.11
119	1,1'-Biphenyl, 3-chloro-	2051-61-8	0.036	0.006
120	3-Octanol, 6-ethyl-	19781-27-2	0.0060	0.0052
121	Hexadecane, 7,9-dimethyl-	21164-95-4	0.0083	0.0075
122	Tetradecane, 4,11-dimethyl-	55045-12-0	0.0099	0.0020
123	Pentadecane, 2-methyl-	1560-93-6	0.0071	0.0062
124	Cyclohexane, octyl-	1795-15-9	0.022	0.028
125	6-Dodecanone	6064-27-3	0.035	0.032
126	6-Dodecanol	6836-38-0	0.014	0.004
127	Hexadecane	544-76-3	0.073	0.024
128	2-Tetradecanone	2345-27-9	0.032	0.009
129	Undecane, 4,6-dimethyl-	17312-82-2	0.014	0.006
130	6-Dodecanone	6064-27-3	0.011	0.004
131	Heptadecane	629-78-7	0.0049	0.0084
132	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.0073	0.0068
133	Tetradecanoic acid	544-63-8	0.022	0.020
134	Nonadecane, 9-methyl-	13287-24-6	0.0079	0.0069
135	Benzenesulfonamide, N-butyl-	3622-84-2	0.018	0.001
136	Pentadecanoic acid	1002-84-2	0.0049	0.0085
137	Hexanedioic acid, mono(2-ethyhexyl) ester	4337-65-9	0.010	0.017
138	Hexadecanoic acid	57-10-3	0.0065	0.0113
139	Isopropyl Palmitate	142-91-6	0.012	0.001
Sum of Tentatively Identified Compounds:			6.35	

WHC-SD-WM-ER-438 REV. 1

1 CAS = Chemical Abstract Service.

2 Average of 3 TST, 1-L samples by ORNL

Table 4-8
 Tank B-103 Tentatively Identified Organic Compounds
 Sorted Alphanumerically --
 Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
53	.alpha.-Methylstyrene	98-83-9	0.0091	0.0079
5	1-Propene, 2-methyl-	115-11-7	0.037	0.010
42	1-Heptene	592-76-7	0.013	0.012
86	1-Undecene	821-95-4	0.014	0.002
60	1-Hexanol, 2-ethyl-	104-76-7	0.049	0.008
3	1-Propene, 2-methyl-	115-11-7	0.078	0.009
66	1-Octanol	111-87-5	0.0062	0.0055
12	1-Propanol	71-23-8	0.10	0.02
9	1-Pentene	109-67-1	0.0050	0.0087
50	1-Hexanol, 2-ethyl-	104-76-7	0.011	0.018
57	1-Decene	872-05-9	0.016	0.003
51	1-Heptanol	111-70-6	0.030	0.003
119	1,1'-Biphenyl, 3-chloro-	2051-61-8	0.036	0.006
44	1,5-Pentanediol, dinitrate	3457-92-9	0.028	0.001
27	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0067	0.0059
70	2-Nonanone	821-55-6	0.0062	0.0054
20	2-Heptene	592-77-8	0.021	0.003
65	2-Heptanone, 6-methyl-	928-68-7	0.0097	0.0018
21	2-Heptene, (E)-	14686-13-6	0.021	0.019
61	2-Pentene, 4,4-dimethyl-, (E) & others		0.013	0.001
48	2-Heptanone, 6-methyl-	928-68-7	0.11	0.01
47	2-Pentene, 2,4-dimethyl-	625-65-0	0.037	0.002
15	2-Butanone	78-93-3	0.044	0.009
128	2-Tetradecanone	2345-27-9	0.032	0.009
95	2(3H)-benzofuranone, 3a,4,5,6-tetrahydro-3a, 6,6-trimethyl	16778-26-0	0.021	0.005
46	2,2'-Bioxepane	74793-02-5	0.036	0.002

WHC-SD-WM-ER-438 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
43	2,5-Pyrrolidinedione, 1-methyl-	1121-07-9	0.028	0.001
14	3-Buten-2-one	78-94-4	0.022	0.002
117	3-Tridecanone	1534-26-5	0.061	0.013
19	3-Heptene	592-78-9	0.026	0.007
67	3-t-Pentylcyclopentanone and others		0.011	0.003
120	3-Octanol, 6-ethyl-	19781-27-2	0.0060	0.0052
96	3-Undecanone & undecanenitrile		0.0089	0.0079
38	3-Heptanone	106-35-4	0.084	0.004
39	3-Heptanol	589-82-2	0.070	0.002
54	3-Heptene, 4-propyl-	4485-13-6	0.0042	0.0073
108	3-Dodecanone	1534-27-6	0.020	0.020
45	4-Heptanone, 3-methyl-	15726-15-5	0.020	0.001
64	5-Undecene, (Z)-	764-96-5	0.0099	0.0012
116	5-Decanol	5205-34-5	0.025	0.007
49	5-Decene, (E)-	7433-56-9	0.015	0.014
125	6-Dodecanone	6064-27-3	0.035	0.032
130	6-Dodecanone	6064-27-3	0.011	0.004
126	6-Dodecanol	6836-38-0	0.014	0.004
115	6-Tridecanone	22026-12-6	0.069	0.013
40	Benzene, 1,3-dimethyl-	108-38-3	0.015	0.001
135	Benzenesulfonamide, N-butyl-	3622-84-2	0.018	0.001
73	Benzoic acid, 2-[(trimethylsilyl)oxyl]-, trimethylsilyl ester	3789-85-3	0.021	0.019
7	Butane, 2-methyl-	78-78-4	0.031	0.002
4	Butane	106-97-8	0.15	0.02
55	Butanoic acid, butyl ester	109-21-7	0.033	0.004
83	C6-cyclohexane		0.031	0.005
101	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.0039	0.0068
111	Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	54965-05-8	0.091	0.017

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
92	Cyclohexane, 1,1'-(1-methylethylidene)bis-	54934-90-6	0.023	0.001
33	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.0032	0.0056
102	Cyclohexane, (1,2-dimethylbutyl)-		0.0055	0.0048
94	Cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.033	0.004
88	Cyclohexane, octyl	1795-15-9	0.10	0.01
87	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.054	0.004
124	Cyclohexane, octyl-	1795-15-9	0.022	0.028
89	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.012	0.010
82	Cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.033	0.004
100	Cyclohexane,(2-ethyl-1-methylbutylidene)-	74810-41-6	0.0086	0.0084
34	Cyclopentanone, 2,2,5-trimethyl-	4573-09-5	0.0097	0.0086
22	Cyclopropane, butyl-	930-57-4	0.021	0.001
1	Cyclopropane	75-19-4	0.056	0.017
52	Cyclotetrasiloxane, octamethyl	556-67-2	0.11	0.04
31	Cyclotrisiloxane, hexamethyl	541-05-9	0.033	0.008
78	Decane, 3-methyl-	13151-34-3	0.018	0.002
79	Decane, 3,8-dimethyl-	17312-55-9	0.016	0.002
58	Decane, 4-methyl-	2847-72-5	0.0096	0.0015
107	Dodecane, 4,6-dimethyl-	61141-72-8	0.43	0.06
90	Dodecane, 4-methyl-	6117-97-1	0.036	0.005
103	Dodecane, 2,5-dimethyl-	56292-65-0	0.031	0.006
6	Ethanol	64-17-5	0.039	0.012
35	Ethylbenzene	100-41-4	0.016	0.001
18	Formic acid, butyl ester	592-84-7	0.012	0.011
29	Furan, tetrahydro-2,4-dimethyl-, trans	39168-02-0	0.014	0.001
17	Furan, tetrahydro-	109-99-9	0.034	0.003
131	Heptadecane	629-78-7	0.0049	0.0084
41	Heptanal	111-71-7	0.018	0.005
25	Heptane, 3-methyl-	589-81-1	0.048	0.001

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
132	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.0073	0.0068
127	Hexadecane	544-76-3	0.073	0.024
121	Hexadecane,7,9-dimethyl-	21164-95-4	0.0083	0.0075
138	Hexadecanoic acid	57-10-3	0.0065	0.0113
28	Hexanal	66-25-1	0.0058	0.0100
137	Hexanedioic acid, mono(2-ethylhexyl) ester	4337-65-9	0.010	0.017
69	Hexyl n-valerate	1117-59-5	0.017	0.001
2	Isobutane	75-28-5	0.0055	0.0095
139	Isopropyl Palmitate	142-91-6	0.012	0.001
10	Methyl nitrate	598-58-3	0.014	0.012
74	n-Amylcyclohexane	4292-92-6	0.021	0.003
75	Naphthalene, decahydro-2-methyl-	2958-76-1	0.011	0.001
63	Nitric acid, pentyl ester	1002-16-0	0.12	0.04
23	Nitric acid, propyl ester	627-13-4	0.090	0.015
59	Nitric acid, hexyl ester	20633-11-8	0.014	0.002
32	Nitric acid, butyl ester	928-45-0	0.13	0.01
16	Nitric acid, ethyl ester	625-58-1	0.092	0.019
134	Nonadecane, 9-methyl-	13287-24-6	0.0079	0.0069
71	Nonanal	124-19-6	0.025	0.005
81	Nonanenitrile	2243-27-8	0.023	0.003
68	Nonanenitrile	2243-27-8	0.021	0.003
80	Nonanol	28473-21-4	0.0069	0.0120
56	Octanal	124-13-0	0.018	0.006
37	p-Xylene	106-42-3	0.043	0.006
118	Pentadecane	629-62-9	0.31	0.11
123	Pentadecane, 2-methyl-	1560-93-6	0.0071	0.0062
136	Pentadecanoic acid	1002-84-2	0.0049	0.0085
11	Pentane, 2-methyl-	107-83-5	0.039	0.001
13	Pentane, 3-methyl-	96-14-0	0.0046	0.0080

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
36	Pentane, 2,3-dimethyl-	565-59-3	0.033	0.002
24	Propane, 2-methyl-2-nitro-	594-70-7	0.022	0.002
30	Tetrachloroethylene	127-18-4	0.036	0.001
106	Tetradecane, 4-methyl-	25117-24-2	0.064	0.012
114	Tetradecane, 3-methyl-	18435-22-8	0.029	0.002
109	Tetradecane	629-59-4	0.72	0.13
122	Tetradecane, 4,11-dimethyl-	55045-12-0	0.0099	0.0020
113	Tetradecane, 4-methyl-	25117-24-2	0.021	0.004
133	Tetradecanoic acid	544-63-8	0.022	0.020
26	trans-1-Butyl-2-methylcyclopropane	38851-70-6	0.0036	0.0063
8	Trichlorofluoromethane	75-69-4	0.25	0.11
99	Tridecane, 6-methyl-	13287-21-3	0.12	0.02
110	Tridecane, 4,8-dimethyl-	55030-62-1	0.096	0.010
98	Tridecane, 7-methyl-	26730-14-3	0.024	0.006
112	Tridecane, 7-methyl-	26730-14-3	0.0081	0.0071
104	Tridecane, 4-methyl-	26730-12-1	0.12	0.02
105	Tridecane, 2-methyl-	1560-96-9	0.075	0.012
93	Tridecane, 7-methyl-	26730-14-3	0.26	0.03
62	Tridecane, 4-methyl-	26730-12-1	0.0067	0.0061
91	Undecane, 2,10-dimethyl-	17301-27-8	0.048	0.006
84	Undecane, 2,6-dimethyl-	17301-23-4	0.15	0.02
77	Undecane, 4-methyl-	2980-69-0	0.010	0.002
76	Undecane, 6-methyl-	17302-33-9	0.011	0.002
129	Undecane, 4,6-dimethyl-	17312-82-2	0.014	0.006
97	Undecane, 4,8-dimethyl-	17301-33-6	0.012	0.003
85	Undecane, 2,4-dimethyl-	17312-80-0	0.030	0.005
72	Undecane, 2-methyl-	7045-71-8	0.013	0.001

1 CAS = Chemical Abstract Service.

2 Average of 3 TST, 1-L samples by ORNL, values listed are estimates.

Table 4-9
 Tank B-103 Tentatively Identified Organic Compounds
 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)
109	Tetradecane	629-59-4	0.72	0.13
107	Dodecane, 4,6-dimethyl-	61141-72-8	0.43	0.06
118	Pentadecane	629-62-9	0.31	0.11
93	Tridecane, 7-methyl-	26730-14-3	0.26	0.03
8	Trichlorofluoromethane	75-69-4	0.25	0.11
84	Undecane, 2,6-dimethyl-	17301-23-4	0.15	0.02
4	Butane	106-97-8	0.15	0.02
32	Nitric acid, butyl ester	928-45-0	0.13	0.01
63	Nitric acid, pentyl ester	1002-16-0	0.12	0.04
104	Tridecane, 4-methyl-	26730-12-1	0.12	0.02
99	Tridecane, 6-methyl-	13287-21-3	0.12	0.02
52	Cyclotetrasiloxane, octamethyl	556-67-2	0.11	0.04
48	2-Heptanone, 6-methyl-	928-68-7	0.11	0.01
12	1-Propanol	71-23-8	0.10	0.02
88	Cyclohexane, octyl-	1795-15-9	0.10	0.01
110	Tridecane, 4,8-dimethyl-	55030-62-1	0.096	0.010
16	Nitric acid, ethyl ester	625-58-1	0.092	0.019
111	Cyclohexane, 1,1,3- trimethyl-2- (3-methylpentyl)-	54965-05-8	0.091	0.017
23	Nitric acid, propyl ester	627-13-4	0.090	0.015
38	3-Heptanone	106-35-4	0.084	0.004
3	1-Propene, 2-methyl-	115-11-7	0.078	0.009
105	Tridecane, 2-methyl-	1560-96-9	0.075	0.012
127	Hexadecane	544-76-3	0.073	0.024
39	3-Heptanol	589-82-2	0.070	0.002
115	6-Tridecanone	22026-12-6	0.069	0.013
106	Tetradecane, 4-methyl-	25117-24-2	0.064	0.012

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
117	3-Tridecanone	1534-26-5	0.061	0.013
1	Cyclopropane	75-19-4	0.056	0.017
87	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.054	0.004
60	1-Hexanol, 2-ethyl-	104-76-7	0.049	0.008
91	Undecane, 2,10-dimethyl-	17301-27-8	0.048	0.006
25	Heptane, 3-methyl-	589-81-1	0.048	0.001
15	2-Butanone	78-93-3	0.044	0.009
37	p-Xylene	106-42-3	0.043	0.006
11	Pentane, 2-methyl-	107-83-5	0.039	0.001
6	Ethanol	64-17-5	0.039	0.012
47	2-Pentene, 2,4-dimethyl-	625-65-0	0.037	0.002
5	1-Propene, 2-methyl-	115-11-7	0.037	0.010
46	2,2'-Bioxepane	74793-02-5	0.036	0.002
90	Dodecane, 4-methyl-	6117-97-1	0.036	0.005
30	Tetrachloroethylene	127-18-4	0.036	0.001
119	1,1'-Biphenyl, 3-chloro-	2051-61-8	0.036	0.006
125	6-Dodecanone	6064-27-3	0.035	0.032
17	Furan, tetrahydro-	109-99-9	0.034	0.003
82	Cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.033	0.004
36	Pentane, 2,3-dimethyl-	565-59-3	0.033	0.002
31	Cyclotrisiloxane, hexamethyl	541-05-9	0.033	0.008
94	Cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.033	0.004
55	Butanoic acid, butyl ester	109-21-7	0.033	0.004
128	2-Tetradecanone	2345-27-9	0.032	0.009
7	Butane, 2-methyl-	78-78-4	0.031	0.002
83	C6-cyclohexane		0.031	0.005
103	Dodecane, 2,5-dimethyl-	56292-65-0	0.031	0.006
85	Undecane, 2,4-dimethyl-	17312-80-0	0.030	0.005
51	1-Heptanol	111-70-6	0.030	0.003

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
114	Tetradecane, 3-methyl-	18435-22-8	0.029	0.002
44	1,5-Pentanediol, dinitrate	3457-92-9	0.028	0.001
43	2,5-Pyrrolidinedione, 1-methyl-	1121-07-9	0.028	0.001
19	3-Heptene	592-78-9	0.026	0.007
71	Nonanal	124-19-6	0.025	0.005
116	5-Decanol	5205-34-5	0.025	0.007
98	Tridecane, 7-methyl-	26730-14-3	0.024	0.006
92	Cyclohexane, 1,1'-(1-methylethylidene)bis-	54934-90-6	0.023	0.001
81	Nonanenitrile	2243-27-8	0.023	0.003
124	Cyclohexane, octyl-	1795-15-9	0.022	0.028
14	3-Buten-2-one	78-94-4	0.022	0.002
24	Propane, 2-methyl-2-nitro-	594-70-7	0.022	0.002
133	Tetradecanoic acid	544-63-8	0.022	0.020
22	Cyclopropane, butyl-	930-57-4	0.021	0.001
74	n-Amylcyclohexane	4292-92-6	0.021	0.003
20	2-Heptene	592-77-8	0.021	0.003
68	Nonanenitrile	2243-27-8	0.021	0.003
21	2-Heptene, (E)-	14686-13-6	0.021	0.019
73	Benzoic acid, 2-[(trimethylsilyl)oxyl]-, trimethylsilyl ester	3789-85-3	0.021	0.019
113	Tetradecane, 4-methyl-	25117-24-2	0.021	0.004
95	2(3H)-benzofuranone, 3a,4,5,6-tetrahydro-3a, 6,6-trimethyl-	16778-26-0	0.021	0.005
45	4-Heptanone, 3-methyl-	15726-15-5	0.020	0.001
108	3-Dodecanone	1534-27-6	0.020	0.020
135	Benzenesulfonamide, N-butyl-	3622-84-2	0.018	0.001
78	Decane, 3-methyl-	13151-34-3	0.018	0.002
56	Octanal	124-13-0	0.018	0.006
41	Heptanal	111-71-7	0.018	0.005
69	Hexyl n-valerate	1117-59-5	0.017	0.001

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
79	Decane, 3,8-dimethyl-	17312-55-9	0.016	0.002
35	Ethylbenzene	100-41-4	0.016	0.001
57	1-Decene	872-05-9	0.016	0.003
40	Benzene, 1,3-dimethyl-	108-38-3	0.015	0.001
49	5-Decene, (E)-	7433-56-9	0.015	0.014
86	1-Undecene	821-95-4	0.014	0.002
29	Furan, tetrahydro-2, 4-dimethyl-, trans	39168-02-0	0.014	0.001
126	6-Dodecanol	6836-38-0	0.014	0.004
129	Undecane, 4,6-dimethyl-	17312-82-2	0.014	0.006
10	Methyl nitrate	598-58-3	0.014	0.012
59	Nitric acid, hexyl ester	20633-11-8	0.014	0.002
72	Undecane, 2-methyl-	7045-71-8	0.013	0.001
42	1-Heptene	592-76-7	0.013	0.012
61	2-Pentene, 4,4-dimethyl-, (E) & others		0.013	0.001
18	Formic acid, butyl ester	592-84-7	0.012	0.011
139	Isopropyl Palmitate	142-91-6	0.012	0.001
89	Cyclohexane, 2-butyl-1, 1,3-trimethyl-	54676-39-0	0.012	0.010
97	Undecane, 4,8-dimethyl-	17301-33-6	0.012	0.003
67	3-t-Pentylcyclopentanone and others		0.011	0.003
76	Undecane, 6-methyl-	17302-33-9	0.011	0.002
75	Naphthalene, decahydro-2-methyl-	2958-76-1	0.011	0.001
130	6-Dodecanone	6064-27-3	0.011	0.004
50	1-Hexanol, 2-ethyl-	104-76-7	0.011	0.018
77	Undecane, 4-methyl-	2980-69-0	0.010	0.002
137	Hexanedioic acid, mono(2-ethylhexyl) ester	4337-65-9	0.010	0.017
122	Tetradecane, 4,11-dimethyl-	55045-12-0	0.0099	0.0020
64	5-Undecene, (Z)-	764-96-5	0.0099	0.0012
34	Cyclopentanone, 2,2,5-trimethyl-	4573-09-5	0.0097	0.0086
65	2-Heptanone, 6-methyl-	928-68-7	0.0097	0.0018

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
58	Decane, 4-methyl-	2847-72-5	0.0096	0.0015
53	.alpha.-Methylstyrene	98-83-9	0.0091	0.0079
96	3-Undecanone & undecanenitrile		0.0089	0.0079
100	Cyclohexane, (2-ethyl-1-methylbutylidene)-	74810-41-6	0.0086	0.0084
121	Hexadecane, 7,9-dimethyl-	21164-95-4	0.0083	0.0075
112	Tridecane, 7-methyl-	26730-14-3	0.0081	0.0071
134	Nonadecane, 9-methyl-	13287-24-6	0.0079	0.0069
132	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.0073	0.0068
123	Pentadecane, 2-methyl	1560-93-6	0.0071	0.0062
80	Nonanol	28473-21-4	0.0069	0.0120
62	Tridecane, 4-methyl-	26730-12-1	0.0067	0.0061
27	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0067	0.0059
138	Hexadecanoic acid	57-10-3	0.0065	0.0113
70	2-Nonanone	821-55-6	0.0062	0.0054
66	1-Octanol	111-87-5	0.0062	0.0055
120	3-Octanol, 6-ethyl-	19781-27-2	0.0060	0.0052
28	Hexanal	66-25-1	0.0058	0.0100
102	Cyclohexane, (1,2-dimethylbutyl)-		0.0055	0.0048
2	Isobutane	75-28-5	0.0055	0.0095
9	1-Pentene	109-67-1	0.0050	0.0087
131	Heptadecane	629-78-7	0.0049	0.0084
136	Pentadecanoic acid	1002-84-2	0.0049	0.0085
13	Pentane, 3-methyl-	96-14-0	0.0046	0.0080
54	3-Heptene, 4-propyl-	4485-13-6	0.0042	0.0073
101	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.0039	0.0068
26	trans-1-Butyl-2-methylcyclopropane	38851-70-6	0.0036	0.0063
33	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.0032	0.0056

1 CAS = Chemical Abstract Service.

2 Average of 3 TST, 1-L samples by ORNL, values listed are estimates.

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