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TANK 241C109 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
8/1994

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

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ECN

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15. Design Verification Required

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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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Cog. Mgr. T. J. Kelley <i>TJ Kelley</i>	<i>9/25/95</i>	QA	
QA		Safety	
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WHC Information Release Administration Specialist:

Kara Broz

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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-C-109 Headspace Gas and Vapor Characterization Results for Samples Collected in August 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
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
OGIST	Oregon Graduate Institute of Science and Technology
ORNL	Oak Ridge National Laboratory
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-C-109 Headspace Gas and Vapor Characterization Results
for Samples Collected in August 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank C-109 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 August 1994 sampling event, but also includes selected results of the July 1993 sampling event. The tank C-109 headspace was sampled in June 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in August 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). However, current governing operating specifications for Watchlist tanks, such as tank C-109, 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 C-109 was vapor sampled in June 1994 using the *in situ* sampling (ISS) method, and again in August 1994 using the more robust vapor sampling system (VSS) method. All sorbent trap samples from the June 1994 ISS event were contaminated with radiological particles, and were not analyzed. Other samples from the June 1994 ISS event are not considered to be equivalent to those from the VSS sampling event (Huckaby and Babad 1995). Furthermore, there are other 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. Results presented here are all from the August 1994 VSS sampling event. Pingel (1994) provides field sampling information for the tank C-109 June 1994 ISS event, and Clauss et al. (1995) provide sample analysis results for the June 1994 ISS method samples.

1.4 Tank Headspace Dynamics

Tank C-109 is the last tank in a 3-tank cascade with tanks C-107 and C-108. It is connected to tank C-108 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade line. Tanks C-107 and C-108 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 C-107 or tank C-108 may be transferred to tank C-109 (unless the cascade lines are obstructed). The possibility that tank C-109 was ventilated primarily via its cascade line to tank C-108 is discussed in Section 3.4.

The cascade of tanks C-107, C-108, and C-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

Headspace gas and vapor samples were collected from tank C-109 using the vapor sampling system (VSS) on August 10, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by the sample and analysis plan¹ (WHC 1995b, Appendix A). The tank headspace temperature was determined to be 27 °C. Air from the tank C-109 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 4, 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), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories. The 39 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 16 trip 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).

¹ The current requirement that sampling and analysis parameters be specified by a tank characterization plan was not in effect for gas and vapor sampling until October 1, 1994.

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,2} 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 were prepared and analyzed by PNL. PNL results were produced at PNL quality assurance impact level 3. SUMMATM canisters were prepared and analyzed by OGIST. OGIST was not operating under a WHC-approved quality assurance plan when samples were analyzed, so OGIST data have been placed in square brackets both in Table 3-1 and elsewhere in the report to indicate that they represent secondary results. Reports by Pool et al. (1995) and Rasmussen (1994) describe sample preparation and analyses.

PNL analyses of inorganic vapor sorbent traps were performed within 15 days after sample collection (Ligotke 1995). OGIST began analysis of SUMMATM canister samples 9 days after they were collected. These are both within the administratively chosen 60-day holding time specified in the WHC quality assurance project plan (Keller 1994). It should be noted that while no holding time study has been performed to address the stability of the target analytes in SUMMATM canisters, the inorganic compounds (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results would probably not be affected even for holding times greater than 60 days.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The average ammonia concentration in tank C-109 ammonia sorbent trap samples was 10.1 ppmv. Ammonia concentrations are typically higher than this level in the passively ventilated waste tank headspaces. The relatively low ammonia concentration in tank C-109 may be related to the fact that only a small quantity of relatively cool waste is stored in tank C-109. Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 10.1 ppmv corresponds to about 0.007 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

OGIST determined the average hydrogen concentration in 3 SUMMATM canister samples to be [125 ppmv]. In general, hydrogen is of concern as a fuel. The measured [125 ppmv] of hydrogen in tank C-109, however, represents only about 0.3 % of the lower flammability limit (LFL) for hydrogen in air, and is not a flammability concern at this level.

Nitrous oxide was determined to be an average of [369 ppmv] in the 3 OGIST SUMMATM canister samples from tank C-109. While this is higher than typical for the passively ventilated tanks that have been sampled, higher nitrous oxide concentrations have been measured. 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 C-109 headspace.

² SUMMA is a trademark of Molectrics, Inc., Cleveland, Ohio.

3.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration measured by OGIST, [3 ppmv], is markedly lower than normal ambient air concentrations, and is the lowest measured in any waste tank. Ambient air typically contains between 350 and 400 ppmv of carbon dioxide. 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.

Carbon monoxide in the tank C-109 headspace, at about [0.41 ppmv], is at a higher concentration than is usually found in ambient air, where it typically ranges from 0.05 to 0.15 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common (e.g., carbon monoxide concentration in tank C-103³ was [26.7 ppmv], Huckaby and Story 1994), and 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 C-109 headspace were determined to be 0.51 ppmv and $\leq$ 0.06 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-109. 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 C-109 headspace.

The water vapor concentration of tank C-109 was determined to be about 20.4 mg/L, at the tank headspace temperature of 27 °C and pressure of 992 mbar (744 torr), (WHC 1995b). This corresponds to water vapor partial pressure of 28.2 mbar (21.2 torr), to a dew point of 23.1 °C, and to a relative humidity of 79 %.

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 Analytes

Aside from water vapor, the most abundant waste constituents in the tank C-109 headspace are nitrous oxide and hydrogen. These, with ammonia, have been detected in most of the passively ventilated tanks that have been sampled in roughly the concentrations measured in tank C-109. While the concentration of nitrous oxide is somewhat higher than typical, the ammonia concentration is relatively low.

The small 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 nitrous oxide results, to 18 % for nitric oxide 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,

³ The carbon monoxide measurement in tank C-103 was made by OGIST, and should be considered secondary data.

dilutions, etc.), and the small relative standard deviations suggest a high degree of control was maintained both in the field and in the laboratories.

Selected headspace characterization data from tanks C-107, C-108, and C-109 are given in Table 3-2 for comparison. The data presented for tanks C-108 and C-109 (which are connected via a cascade line) do not conclusively indicate whether the tanks breathe independently or not, however, the data are consistent with the premise that tank C-109 breathes primarily via its cascade line with tank C-108. This would also explain the very low level of carbon dioxide in tank C-109.

4.0 ORGANIC VAPORS

Organic vapors in the tank C-109 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both laboratories 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. (1994) and Pool et al. (1995). Quantitative measurements of the methane concentration and total nonmethane organic carbon (TNMOC) concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method were also performed by OGIST (EPA 1988, Rasmussen 1994).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-109. PNL results were produced at PNL quality assurance impact level 3. All PNL SUMMA™ canister analyses were completed within 59 days after sample collection. This satisfies the administratively chosen 60-day holding time of 60 days (Keller 1994). However, no holding time study has been performed to address organic compound stability in SUMMA™ canisters in the typical chemical matrix of the tank headspace 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. 1994). 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 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 40 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.

Given in Table 4-1 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL and OGIST. PNL performed analyses according to the EPA TO-14 methodology (EPA 1988, Pool et al. 1995). Only 1 of the 40 TO-14 analytes was observed to be above the 0.002 ppmv quantitation limit of the analyses. The results for methane are those of OGIST (Rasmussen 1994). Averages reported are from analyses of 3 SUMMA™ canister samples

ORNL positively identified 17 of 27 analytes selected by WHC. 1-Butanol was the only analyte that was quantitatively measured in all 4 of the TST samples, all others being measured outside the instrumental calibration range. The positively identified analytes, and their average concentrations from the analysis of 4 TSTs, are given in Tables 4-2 and 4-3. Two compounds, butanal and 1-butanol, have been listed in Table 4-3 to indicate their measurements were not performed within their practical holding times (Jenkins 1995b).

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 4-3, the analyses of butanal and 1-butanol exceeded their practical holding times, and may have been affected by the 25 day period between sample collection and analysis. Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the practical holding times of butanal and 1-butanol are 1 and 17 days, respectively. It should be noted that the contractual holding time for the TST samples was 60 days (Keller 1994).

Three target analytes were common to both the ORNL and PNL analyses: Dichloromethane, benzene, and toluene. Neither ORNL nor PNL detected dichloromethane. ORNL detected trace amounts of benzene and toluene, but these were both below the 0.002 ppmv PNL limit of detection. The PNL and ORNL results for these 2 compounds are listed in Table 4-4 for comparison.

The 2 most abundant analytes in Tables 4-1 through 4-3 are methane and ethanenitrile. At [0.927 ppmv], the methane concentration in tank C-109 is above ambient levels, which are typically about 0.2 ppmv. Elevated methane concentrations have been observed in other waste tank headspaces, and methane is probably formed during the chemical and radiolytic degradation of organic wastes. For methane, 1 ppmv corresponds to roughly 0.002 % of its LFL. Ethanenitrile, at 0.26 ppmv, similarly presents virtually no flammable risk.

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 standards of 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 SUMMATM 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 SUMMATM samples has been problematic.

The tentatively identified compounds recovered from SUMMATM samples, in the order by which the eluted chromatographically, are given in Table 4-5 with estimated concentrations. 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 4-6. Compounds are listed in Table 4-6 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-6 are all 4-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. Because the list of tentatively identified organic compounds in TST samples is particularly long and locating any given compound may be difficult, the list has been sorted alphanumerically by compound name in Table 4-7. Table 4-8 gives the same list, sorted in order of decreasing estimated concentration. Numbers in the first columns of Tables 4-7 and 4-8 (Cmpd #) identify the location of the compound in Table 4-6. Estimated concentrations are in mg/m^3 , based on dry air at 0 °C and 1.01 bar.

The PNL and ORNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Pool et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-5 through 4-8 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. Results in Tables 4-5 through 4-8 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 12 and 13 in Table 4-6). 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 using the EPA TO-12 method (Rasmussen 1994). The sample mean was $[0.65 \text{ mg}/\text{m}^3]$, with a standard deviation of $[0.03 \text{ mg}/\text{m}^3]$. This value is low compared to most other waste tanks sampled to date. The TNMOC concentration in clean ambient air may range from 0.030 to 0.100 mg/m^3 .

4.4 Discussion of Organic Analytes

Some of the compounds listed in Tables 4-1 through 4-8 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 tributyl phosphate, which was used as an extractant in several Hanford processes; dibutyl butylphosphonate, which was a contaminant of tributyl phosphate; and the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-undecane, n-dodecane, n-tridecane, and n-pentadecane) that were used as diluents for tributyl phosphate. Notably absent from the tank C-109 headspace are the semivolatile cyclic alkanes (e.g., methylated decahydronaphthalenes, cyclopentanes, and cyclohexanes) that have been observed in the 241-BY tank farm and several 241-C farm tanks.

Most of the compounds in Tables 4-1 through 4-8 are believed to be chemical 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 NPHs.

Examination of the compounds listed in Tables 4-1 through 4-8 suggests many of the volatile species (presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom. For example, most alcohols are 1-alkanols, and ketones generally have the double bonded oxygen atom on the second carbon atom.

Though their concentrations are not significant, many alcohols and acids were tentatively identified in TST samples by ORNL. 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.

5.0 SUMMARY

The tank C-109 headspace was sampled in August 1994 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.
- 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.
- Clauss, T.W., Pool, K. H., M. W. Ligothe, R. B. Lucke, B. D. McVeety, G. S. Klinger, A.K. Sharma, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1995, *Vapor Space Characterization of Waste Tank 241-C-109: Results from Samples Collected on 6/23/94*, PNL-10366 UC-606, Pacific Northwest Laboratory, 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.
- 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., 1994a, *Vapor Sampling System (VSS) and In Situ Sampling (ISS) Method Comparison*, WHC-SD-WM-RPT-101 Rev. 0, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., 1994b, *Tank 241-C-103 Headspace Flammability*, WHC-EP-0734 Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Huckaby, J. L., 1995a, *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.
- Huckaby, J. L., 1995b, *Tank 241-C-108 Headspace Gas and Vapor Characterization Results for Samples Collected in July 1993 and August 1994*, WHC-SD-WM-ER-464 Rev. 2, 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 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 090195A 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. E. Higgins, C. Y. Ma, and J. T. Skeen, 1994, *Analysis of Tank 241-C-109 Headspace Components*, 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, 1995, *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.
- Ligotke, M. W. 1995, *PNL Vapor Project Analytical Holding Times*, (Letter to D. R. Bratzel, September 23), 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.
- 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.
- Pingel, L. A., 1994, *Results from the In-Situ Vapor Sampling of Waste Tank C-109*, (Internal memorandum 8E920-SAS94-106 to J. L. Huckaby), Westinghouse Hanford Company, Richland, Washington.
- Pool, K. H., T. W. Clauss, M. W. Ligotke, R. B. Lucke, B. D. McVeety, A. K. Sharma, M. McCulloch, J. S. Fruchter, and S. C. Goheen, 1994, *Vapor Space Characterization of Waste Tank 241-C-109: Results from Samples Collected on 8/10/94*, PNL-10418 UC-606, Pacific Northwest Laboratory, Richland, Washington.
- Rasmussen, R. A., 1994, *Oregon Graduate Institute Vapor Analysis Results, Tank 241-C-109, August 1994*, Oregon Graduate Institute of Science and Technology, Beaverton, Oregon.

WHC-SD-WM-ER-424 REV. 2

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-C-109 Using the Vapor Sampling System*, WHC-SD-WM-RPT-111, Westinghouse Hanford Company, Richland, Washington.

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Table 2-1
Tank C-109 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	1.0	Organic vapors	4 tank air samples
		4.0	Organic vapors	4 tank air samples + 2 trip blanks
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous Oxide, Carbon Dioxide, Carbon Monoxide	3 tank air samples
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
	SUMMA™ canister	6.0	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 C-109 Inorganic Gas and Vapor Concentrations --
Analyses by Oregon Graduate Institute of Science and Technology and by Pacific Northwest Laboratory

Compound	CAS ¹ number	Sample Type	Number of samples	Average ² (ppmv)	Standard Deviation ² (ppmv)	RSD ^{2,3} (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	10.1	0.8	8
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	[3]	[≤ 0.3]	[≤ 10]
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	[0.41]	[0.01]	[2]
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	[125]	[0.6]	[0.5]
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.51	0.09	18
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.06	—	—
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	[369]	[2]	[0.6]
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	28,400 (20.4 mg/L)	1,100 (0.8 mg/L)	4

1 CAS = Chemical Abstracts Service.

2 Bracketed values are from OGIST and should be considered secondary results, non-bracketed values are from PNL and should be considered primary results.

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

Table 3-2
Comparison of Tank C-107, C-108, and C-109 Headspace Constituents --
Inorganic Analyses by Oregon Graduate Institute of Science and Technology,
and Organic Analyses by Oak Ridge National Laboratory¹

Tank:	C-107	C-108 ²	C-109 ³
Date sampled, (mo/day/yr)	9/9/94	8/5/94	8/10/94
Headspace temperature, (°C)	45.9	25	27
Ammonia, (ppmv)	84	2.7	10.1
Hydrogen, (ppmv)	[230]	[15.3]	[125]
Carbon dioxide, (ppmv)	[725]	[16.3]	[3]
Carbon monoxide, (ppmv)	[1.7]	[0.10]	[0.41]
Nitric oxide, (ppmv)	0.20	0.24	0.51
Nitrogen dioxide, (ppmv)	≤ 0.02	≤ 0.04	≤ 0.06
Nitrous oxide, (ppmv)	[78]	[344]	[369]
Water vapor, (mg/m ³)	70.7	17.5	20.4
Water vapor, (% relative humidity)	86	76	79
Ethanenitrile (acetonitrile), (ppmv)	(0.25)	(0.0052)	(0.26)
Propanone (acetone), (ppmv)	(0.094)	0.018	(0.012)
1-Butanol, (ppmv)	(0.0025)	(0.00049)	0.0032
n-Dodecane, (ppmv)	0.0073	(0.00053)	(0.00026)
n-Tridecane, (ppmv)	0.0092	(0.0011)	(0.00047)
Total nonmethane organic compounds by EPA TO-12 method, (mg/m ³)	[3.6]	[0.35]	[0.65]

¹ Where PNL inorganic gas or vapor data were unavailable for tanks C-108 and C-109, OGIST results are given in brackets to indicate the data should be considered secondary results. Organic vapor results are from ORNL, with semiquantitative values in parentheses and quantitative values not in parentheses.

² Data are from Huckaby 1995d.

³ Data are from Huckaby 1994e.

Table 4-1
Tank C-109 Quantitatively Measured Organic Compound Average Concentrations –
Analyses by Pacific Northwest Laboratory

Compound	CAS ¹ number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
Methane ⁴	74-82-8	[0.927]	[0.006]	[0.6]
Trichlorofluoromethane	75-69-4	0.0071	0.00005	0.7

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 %.

4 Methane analyses were performed by OGIST and should be considered a secondary result (Ramussen 1994).

Table 4-2
Tank C-109 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	Ethananitrile (acetonitrile)	75-05-8	0.26	0.04	15
2	Propanone (acetone)	67-64-1	0.012	0.006	53
3	Propanenitrile	107-12-0	0.0013	0.0009	73
4	Benzene	71-43-2	0.00013	0.00012	98
5	n-Butanenitrile	109-74-0	0.00020	0.00014	70
6	2-Pentanone	107-87-9	0.00049	0.00036	73
7	Toluene	108-88-3	0.000019	0.000039	200
8	2-Hexanone	591-78-6	0.00012	0.00009	72
9	n-Octane	111-65-9	0.000069	0.000056	81
10	2-Heptanone	110-43-0	0.000084	0.000057	68
11	n-Nonane	111-84-2	0.00011	0.00006	52
12	2-Octanone	111-13-7	0.000063	0.000042	67
13	n-Nonanenitrile	2243-27-8	0.000010	0.000021	200
14	n-Dodecane	112-70-3	0.00026	0.00006	23
15	n-Tridecane	629-50-5	0.00047	0.00008	18

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 4 TST samples: 1 was 1-L and 3 were 4-L.

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

Table 4-3
Tank C-109 Positively Identified 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	0.0015	0.0010	70
2	1-Butanol ⁶	71-36-3	0.0032	0.0023	71

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples: 1 was 1-L and 3 were 4-L.

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 4-4
Tank C-109 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 (%)
Benzene	71-43-2	0.00013	< 0.002	—
Toluene	108-88-3	0.000019	< 0.002	—

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples; 1 was 1-L and 3 were 4-L.

3 Average of 3 samples.

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

Table 4-5
Tank C-109 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	Ethanenitrile (acetonitrile)	75-05-8	0.15	0.01
2	Propanone (acetone)	67-64-1	0.05	0.00
3	Alkyl nitrate	598-58-3	0.12	0.00
Sum of tentatively identified compounds:			0.31	

1 CAS = Chemical Abstracts Service.

2 Average of 3 samples.

Table 4-6
 Tank C-109 Tentatively Identified Organic Compounds in TST Samples
 in 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	Acetaldehyde and CO ₂		0.007	0.013
2	CO ₂ and argon		0.010	0.020
3	Methane, trichlorofluoro-	75-69-4	0.006	0.012
4	Fluoroethylene	75-02-5	0.412	0.128
5	Nirtic acid, ethyl ester	625-58-1	0.007	0.005
6	Acetic acid	64-19-7	0.018	0.021
7	Nitric acid, propyl ester	627-13-4	0.004	0.005
8	Unknown		0.003	0.004
9	Siloxane		0.003	0.006
10	Hexanal	66-25-1	0.001	0.003
11	Butanoic acid	107-92-6	0.007	0.010
12	Hexamethylcyclotrisiloxane	541-05-9	0.017	0.034
13	Hesamethylcyclotrisiloxane	541-05-9	0.005	0.010
14	Heptanal	111-71-7	0.002	0.001
15	Unknown		0.002	0.001
16	Hexanoic acid	142-62-1	0.002	0.002
17	Cyclotetrasiloxane, octamethyl-	556-67-2	0.020	0.016
18	Octanal	124-13-0	0.005	0.002
19	1-Hexanol, 2-ethyl-	104-76-7	0.002	0.002
20	1-Octanol and alkanoic acid		0.001	0.001
21	Isothiazole	288-16-4	0.001	0.001
22	Ethanone, 1-phenyl-	98-86-2	0.017	0.006
23	Benzenemethanol, .alpha.,.alpha.-dimethyl-	617-94-7	0.011	0.008
24	Nonanal	124-19-6	0.010	0.001
25	2-Nonenal, (E)-	18829-56-6	0.001	0.002
26	Hexanoic acid, 2-ethyl-	149-57-5	0.001	0.001

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.003	0.005
28	2-Dodecenal	4826-62-4	0.001	0.002
29	1-Nonanol	143-08-8	0.001	0.001
30	3-Undecene, (E)- and others		0.001	0.002
31	Decanal	112-31-2	0.009	0.005
32	Perfluorotributylamine	311-89-7	0.021	0.042
33	Benzothiazole	95-16-9	0.001	0.001
34	1,3,5,7-Tetraazatricyclo-[3.3.1.1 ^{3,7}]decane	100-97-0	0.004	0.004
35	Phenol, 4-(1,1-dimethylethyl)-	98-54-4	0.001	0.001
36	Dodecanal	112-54-9	0.001	0.001
37	Alkanoic acid		0.001	0.001
38	Butanoic acid, anhydride and others		0.001	0.001
39	Undecanal	112-44-7	0.002	0.001
40	Alkane and alkanoic acid		0.001	0.001
41	Alkane and others		0.001	0.001
42	Alkane		0.001	0.001
43	Butanoic acid, hexyl ester	2639-63-6	0.001	0.001
44	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.001	0.001
45	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	0.003	0.002
46	Tetradecane	629-59-4	0.004	0.002
47	Dodecanal	112-54-9	0.001	0.001
48	Alkane		0.002	0.001
49	1-Decanol	112-30-1	0.002	0.001
50	1,12-Dodecanediol	5675-51-4	0.001	0.001
51	Undecane, 5-methyl-	1632-70-8	0.001	0.001
52	1-Tetradecanol	112-72-1	0.002	0.001
53	Mixture		0.001	0.002

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
54	Cyclododecane	294-62-2	0.002	0.001
55	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	0.002	0.001
56	Alkane		0.002	0.002
57	Pentadecane	629-62-9	0.001	0.002
58	Dodecanoic acid	143-07-7	0.005	0.002
59	Alkane		0.001	0.001
60	Hexadecane	544-76-3	0.002	0.001
61	Alkanoic acid		0.043	0.004
62	Benzenamine, N-phenyl-	122-39-4	0.008	0.007
63	Alkene and others		0.004	0.002
64	Hexadecane	544-76-3	0.001	0.001
65	Alkane		0.001	0.001
66	Octyl phenol isomer		0.001	0.001
67	Nonylphenol isomer and siloxane		0.001	< 0.001
68	Cyclohexane, 1-(cyclohexyl-methyl)-4-ethyl-cis	54934-95-1	0.003	0.003
69	Mixture		0.001	0.003
70	Tetradecanoic acid	544-63-8	0.046	0.023
71	Alkane		0.001	0.002
72	Alkane		0.002	0.002
73	Benzene, (ethylsulfonyl)-	599-70-2	0.088	0.046
74	Tetradecanoic acid	544-63-8	0.004	0.002
75	Alkene		0.002	0.002
76	Pentadecanoic acid	1002-84-2	0.029	0.015
77	1-Hexadecanol	36653-82-4	0.009	0.007
78	7-Acetyl-1,1,3,4,4,6-hexamethyltetralin	1506-02-1	0.001	< 0.001
79	9-Hexadecenoic acid	2091-29-4	0.047	0.021
80	Hexadecanoic acid	57-10-3	0.100	0.055
81	1-Heptadecanol, acetate and others		0.001	0.001

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
82	1-Nonadecene	18435-45-5	0.001	0.001
83	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.003
84	Mixture		0.001	0.001
85	Alkane		0.005	0.009
Sum of tentatively identified compounds:			1.040	

1 CAS = Chemical Abstracts Service.

2 Average of 4 TST samples: 1 was 1-L and 3 were 4-L, values listed are estimates.

Table 4-7
 Tank C-109 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)
19	1-Hexanol, 2-ethyl-	104-76-7	0.002	0.002
82	1-Nonadecene	18435-45-5	0.001	0.001
81	1-Heptadecanol, acetate and others		0.001	0.001
20	1-Octanol and alkanoic acid		0.001	0.001
49	1-Decanol	112-30-1	0.002	0.001
77	1-Hexadecanol	36653-82-4	0.009	0.007
29	1-Nonanol	143-08-8	0.001	0.001
52	1-Tetradecanol	112-72-1	0.002	0.001
50	1,12-Dodecanediol	5675-51-4	0.001	0.001
34	1,3,5,7-Tetraazatricyclo- [3.3.1.1 ^{3,7}]decane	100-97-0	0.004	0.004
25	2-Nonenal, (E)-	18829-56-6	0.001	0.002
28	2-Dodecenal	4826-62-4	0.001	0.002
55	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	0.002	0.001
30	3-Undecene, (E)- and others		0.001	0.002
78	7-Acetyl-1,1,3,4,4,6-hexamethyltetralin	1506-02-1	0.001	< 0.001
79	9-Hexadecenoic acid	2091-29-4	0.047	0.021
1	Acetaldehyde and CO ₂		0.007	0.013
6	Acetic acid	64-19-7	0.018	0.021
40	Alkane and alkanoic acid		0.001	0.001
41	Alkane and others		0.001	0.001
42	Alkane		0.001	0.001
48	Alkane		0.002	0.001
56	Alkane		0.002	0.002
59	Alkane		0.001	0.001
65	Alkane		0.001	0.001
71	Alkane		0.001	0.002

WHC-SD-WM-ER-424 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
72	Alkane		0.002	0.002
85	Alkane		0.005	0.009
37	Alkanoic acid		0.001	0.001
61	Alkanoic acid		0.043	0.004
63	Alkene and others		0.004	0.002
75	Alkene		0.002	0.002
62	Benzenamine, N-phenyl-	122-39-4	0.008	0.007
73	Benzene, (ethylsulfonyl)-	599-70-2	0.088	0.046
23	Benzenemethanol, .alpha.,.alpha.-dimethyl-	617-94-7	0.011	0.008
27	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.003	0.005
33	Benzothiazole	95-16-9	0.001	0.001
11	Butanoic acid	107-92-6	0.007	0.010
38	Butanoic acid, anhydride and others		0.001	0.001
43	Butanoic acid, hexyl ester	2639-63-6	0.001	0.001
2	CO ₂ and argon		0.010	0.020
54	Cyclododecane	294-62-2	0.002	0.001
68	Cyclohexane, 1-(cyclohexyl-methyl)-4-ethyl-cis	54934-95-1	0.003	0.003
17	Cyclotetrasiloxane, octamethyl-	556-67-2	0.020	0.016
13	Cyclotrisiloxane, hexamethyl-	541-05-9	0.005	0.010
31	Decanal	112-31-2	0.009	0.005
36	Dodecanal	112-54-9	0.001	0.001
47	Dodecanal	112-54-9	0.001	0.001
58	Dodecanoic acid	143-07-7	0.005	0.002
22	Ethanone, 1-phenyl-	98-86-2	0.017	0.006
4	Fluoroethylene	75-02-5	0.412	0.128
14	Heptanal	111-71-7	0.002	0.001
44	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.001	0.001
60	Hexadecane	544-76-3	0.002	0.001

WHC-SD-WM-ER-424 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
64	Hexadecane	544-76-3	0.001	0.001
80	Hexadecanoic acid	57-10-3	0.100	0.055
83	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.003
12	Hexamethylcyclotrisiloxane	541-05-9	0.017	0.034
10	Hexanal	66-25-1	0.001	0.003
16	Hexanoic acid	142-62-1	0.002	0.002
26	Hexanoic acid, 2-ethyl-	149-57-5	0.001	0.001
21	Isothiazole	288-16-4	0.001	0.001
3	Methane, trichlorofluoro-	75-69-4	0.006	0.012
53	Mixture		0.001	0.002
69	Mixture		0.001	0.003
84	Mixture		0.001	0.001
5	Nirtic acid, ethyl ester	625-58-1	0.007	0.005
7	Nitric acid, propyl ester	627-13-4	0.004	0.005
24	Nonanal	124-19-6	0.010	0.001
67	Nonylphenol isomer and siloxane		0.001	< 0.001
18	Octanal	124-13-0	0.005	0.002
66	Octyl phenol isomer		0.001	0.001
57	Pentadecane	629-62-9	0.001	0.002
76	Pentadecanoic acid	1002-84-2	0.029	0.015
32	Perfluorotributylamine	311-89-7	0.021	0.042
35	Phenol, 4-(1,1-dimethylethyl)-	98-54-4	0.001	0.001
45	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	0.003	0.002
9	Siloxane		0.003	0.006
46	Tetradecane	629-59-4	0.004	0.002
70	Tetradecanoic acid	544-63-8	0.046	0.023
74	Tetradecanoic acid	544-63-8	0.004	0.002
39	Undecanal	112-44-7	0.002	0.001

WHC-SD-WM-ER-424 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
51	Undecane, 5-methyl-	1632-70-8	0.001	0.001
8	Unknown		0.003	0.004
15	Unknown		0.002	0.001
Sum of tentatively identified compounds:			1.040	

1 CAS = Chemical Abstracts Service.

2 Average of 4 TST samples: 1 was 1-L and 3 were 4-L, values listed are estimates.

Table 4-8
 Tank C-109 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)
4	Fluoroethylene	75-02-5	0.412	0.128
80	Hexadecanoic acid	57-10-3	0.100	0.055
73	Benzene, (ethylsulfonyl)-	599-70-2	0.088	0.046
79	9-Hexadecenoic acid	2091-29-4	0.047	0.021
70	Tetradecanoic acid	544-63-8	0.046	0.023
61	Alkanoic acid		0.043	0.004
76	Pentadecanoic acid	1002-84-2	0.029	0.015
32	Perfluorotributylamine	311-89-7	0.021	0.042
17	Cyclotetrasiloxane, octamethyl-	556-67-2	0.020	0.016
6	Acetic acid	64-19-7	0.018	0.021
22	Ethanone, 1-phenyl-	98-86-2	0.017	0.006
12	Hexamethylcyclotrisiloxane	541-05-9	0.017	0.034
23	Benzenemethanol, .alpha.,.alpha.-dimethyl-	617-94-7	0.011	0.008
2	CO2 and argon		0.010	0.020
24	Nonanal	124-19-6	0.010	0.001
77	1-Hexadecanol	36653-82-4	0.009	0.007
31	Decanal	112-31-2	0.009	0.005
62	Benzenamine, N-phenyl-	122-39-4	0.008	0.007
5	Nitric acid, ethyl ester	625-58-1	0.007	0.005
11	Butanoic acid	107-92-6	0.007	0.010
1	Acetaldehyde and CO2		0.007	0.013
3	Methane, trichlorofluoro-	75-69-4	0.006	0.012
85	Alkane		0.005	0.009
58	Dodecanoic acid	143-07-7	0.005	0.002
13	Cyclotrisiloxane, hexamethyl-	541-05-9	0.005	0.010
18	Octanal	124-13-0	0.005	0.002
7	Nitric acid, propyl ester	627-13-4	0.004	0.005

WHC-SD-WM-ER-424 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
63	Alkene and others		0.004	0.002
74	Tetradecanoic acid	544-63-8	0.004	0.002
34	1,3,5,7-Tetraazatricyclo- [3.3.1.1 ^{3,7}]decane	100-97-0	0.004	0.004
46	Tetradecane	629-59-4	0.004	0.002
8	Unknown		0.003	0.004
68	Cyclohexane, 1-(cyclohexyl-methyl)-4-ethyl-cis	54934-95-1	0.003	0.003
27	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.003	0.005
9	Siloxane		0.003	0.006
45	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	0.003	0.002
16	Hexanoic acid	142-62-1	0.002	0.002
19	1-Hexanol, 2-ethyl-	104-76-7	0.002	0.002
39	Undecanal	112-44-7	0.002	0.001
75	Alkene		0.002	0.002
72	Alkane		0.002	0.002
14	Heptanal	111-71-7	0.002	0.001
15	Unknown		0.002	0.001
60	Hexadecane	544-76-3	0.002	0.001
56	Alkane		0.002	0.002
55	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-	719-22-2	0.002	0.001
54	Cyclododecane	294-62-2	0.002	0.001
48	Alkane		0.002	0.001
49	1-Decanol	112-30-1	0.002	0.001
52	1-Tetradecanol	112-72-1	0.002	0.001
51	Undecane, 5-methyl-	1632-70-8	0.001	0.001
50	1,12-Dodecanediol	5675-51-4	0.001	0.001
53	Mixture		0.001	0.002
47	Dodecanal	112-54-9	0.001	0.001

WHC-SD-WM-ER-424 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
37	Alkanoic acid		0.001	0.001
38	Butanoic acid, anhydride and others		0.001	0.001
57	Pentadecane	629-62-9	0.001	0.002
36	Dodecanal	112-54-9	0.001	0.001
59	Alkane		0.001	0.001
44	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.001	0.001
43	Butanoic acid, hexyl ester	2639-63-6	0.001	0.001
42	Alkane		0.001	0.001
35	Phenol, 4-(1,1-dimethylethyl)-	98-54-4	0.001	0.001
64	Hexadecane	544-76-3	0.001	0.001
65	Alkane		0.001	0.001
66	Octyl phenol isomer		0.001	0.001
67	Nonylphenol isomer and siloxane		0.001	< 0.001
33	Benzothiazole	95-16-9	0.001	0.001
69	Mixture		0.001	0.003
30	3-Undecene, (E)- and others		0.001	0.002
71	Alkane		0.001	0.002
41	Alkane and others		0.001	0.001
10	Hexanal	66-25-1	0.001	0.003
29	1-Nonanol	143-08-8	0.001	0.001
40	Alkane and alkanoic acid		0.001	0.001
28	2-Dodecenal	4826-62-4	0.001	0.002
26	Hexanoic acid, 2-ethyl-	149-57-5	0.001	0.001
78	7-Acetyl-1,1,3,4,4,6-hexamethyltetralin	1506-02-1	0.001	< 0.001
25	2-Nonenal, (E)-	18829-56-6	0.001	0.002
20	1-Octanol and alkanoic acid		0.001	0.001
81	1-Heptadecanol, acetate and others		0.001	0.001
82	1-Nonadecene	18435-45-5	0.001	0.001
83	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.003

WHC-SD-WM-ER-424 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
84	Mixture		0.001	0.001
21	Isothiazole	288-16-4	0.001	0.001
Sum of tentatively identified compounds:			1.040	

1 CAS = Chemical Abstracts Service.

2 Average of 4 TST samples: 1 was 1-L and 3 were 4-L, values listed are estimates.