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CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
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7. Abstract <p>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.</p>		
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Tank 241-T-111 Headspace Gas and Vapor Characterization Results for Samples Collected in January 1995

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Date Published
September 1995

Prepared for the U.S. Department of Energy
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**Tank 241-T-111 Headspace Gas and Vapor Characterization Results
for Samples Collected in January 1995**

September 14, 1995

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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-T-111 Headspace Gas and Vapor Characterization Results
for Samples Collected in January 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank T-111 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. 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 T-111 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

1.2 Characterization Data Criteria

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

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank T-111, 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 T-111 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 T-111 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 T-111 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank T-111 is the second tank in a 3-tank cascade with tanks T-110 and T-112, and is connected to each of these tanks via 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade lines. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank T-110 or tank T-112 may be transferred to tank T-111 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for either tanks T-110 or T-112 to assess their potential effect on tank T-111.

The cascade of tanks T-110, T-111, and T-112 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 T-111 using the vapor sampling system (VSS) on January 20, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-T-111 Tank Characterization Plan* (Homi 1995). The tank headspace temperature was determined to be 15.4 °C. Air from the tank T-111 headspace was withdrawn via a 6.1 m-long heated sampling probe mounted in riser 3, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All samples were collected between 3:02 p.m. and 8:33 p.m.

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 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 as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM were prepared and analyzed by PNL, with analyses performed within 32 days and 34 days, respectively, of sample collection (Ligotke 1995). These satisfy the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994). All sample preparation and analyses were performed at PNL quality assurance impact level 2 (Klinger et al. 1995).

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Based on analyses of 6 ammonia sorbent trap samples, the average ammonia concentration in the headspace of tank T-111 was computed to be 226 ppmv. This is a typical ammonia concentration for the waste tanks that have been sampled. 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 226 ppmv corresponds to about 0.15 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank T-111 was determined by PNL to be < 94 ppmv. Given that the LFL for hydrogen in air is about 4 vol%, the < 94 ppmv hydrogen concentration in tank T-111 corresponds to < 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank T-111.

The nitrous oxide concentration in tank T-111, measured to be < 12.6 ppmv in each of the 3 SUMMATM samples, is relatively low compared to other waste tanks that have been sampled. Nitrous oxide has been detected in many other passively ventilated waste tanks, and has been measured at concentrations as high as 878 ppmv in tank U-103 (Ligotke et al. 1995). 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 T-111 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide was determined to be < 12 ppmv in the 3 SUMMATM samples from tank T-111. 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. Elevated carbon monoxide concentrations are common in the passively ventilated tanks, and are thought to be due to the decomposition of organic waste. 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 have been placed in brackets to indicate it should be considered secondary data.

The carbon dioxide concentration in the tank T-111 headspace, measured to be an average 69 ppmv, is significantly lower than it is in ambient air. 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 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. The 2 ambient air samples collected at the start of the tank T-111 gas and vapor sampling event, for example, were measured to have an average 374 ppmv of carbon dioxide (Klinger et al. 1995).

3.3 Nitric Oxide, Nitrogen Dioxide, Water, and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank T-111 headspace were determined to be ≤ 0.06 and ≤ 0.09 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank T-111. The measurable presence of nitric oxide is not uncommon in the waste tank headspaces, and 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 T-111 headspace.

The water vapor concentration of tank T-111 was determined to be about 11.8 mg/L, at the measured tank headspace temperature of 15.4 °C and pressure of 995.9 mbar (747.1 torr), (WHC 1995b). This equates to a water vapor partial pressure of 15.7 mbar (11.7 torr), to a dew point of 13.7 °C, and to a relative humidity of 90 %.

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, the most abundant waste constituent in the tank T-111 headspace is ammonia. Ammonia has been detected in all tank headspaces sampled to date. Compared to other passively ventilated waste tanks that have been sampled, tank T-111 has low concentrations of both hydrogen and nitrous oxide.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good for the methods used at the concentrations reported. Relative standard deviations range from less than 1 % for the measurement of ammonia, to about 7 % for the measurement of carbon dioxide. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), 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 T-111 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) detector to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Klinger et al. (1995).

PNL SUMMA™ sample results should be considered to be the primary organic vapor data for tank T-111. All PNL sample preparation and analyses were performed at PNL quality assurance impact level 2. It should be noted that because tank T-111 sample analyses were assigned a low priority by WHC, PNL SUMMA™ canister organic analyses were not performed until 94 days after sample collection (Ligotke 1995), exceeding the administratively chosen 60-day holding time (Keller 1994). No holding time study has been performed to address the stability of organic compounds in SUMMA™ canisters in the chemical matrix of the waste 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 analyses at ORNL were not performed under a WHC approved quality assurance plan, documentation of the quality assurance measures is less rigorous. Results of a quality assurance assessment of ORNL by Hendrickson (1995) should be reviewed before results unique to the TST samples are used for decision making.

ORNL analyzed 4 of the 12 TST tank samples, 1 of the 2 TST field blanks, and 1 of the 2 TST trip blanks. ORNL analyzed a single 4-L TST tank sample to estimate the concentration of organic vapors sampled. Because the measured organic vapor concentrations were higher than optimum for 4-L samples, the 1-L TST tank samples were analyzed for analyte identification and quantification.

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 both means and standard deviations 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 from the analysis of standards. The concentration of an analyte in the sample is said to be quantitatively measured if the response of the GC/MS has been established at several known concentrations of that analyte (i.e., the GC/MS has been calibrated for that analyte), and the MS response to the analyte in the sample is between the lowest and highest responses to the known concentrations (i.e., the analyte is within the calibration range).

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

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples. Methane was analyzed with the inorganic gases (and not by GC/MS). Other SUMMA™ analyses were performed according to the EPA TO-14 methodology by PNL (EPA 1988, Klinger et al. 1995). Of the 39 TO-14 target analytes, only 7 were measured to be at or above the 0.005 ppmv quantitation limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

Jenkins et al. (1995a) report the positive identification of 24 of 27 target analytes in TST samples. 1,1-Dichloroethene, tributyl phosphate, and dibutyl butylphosphonate were the only TST target analytes not detected in the TST samples. The average concentrations of the target analytes, from the analysis of 3 TSTs, are given in Tables 4-2, 4-3, and 4-4. Target analytes for which all of the measured concentrations were within the calibration range of the instrument are listed in Table 4-2, target analytes for which 1 or more of the measured concentrations were outside the calibration range are listed in Table 4-3, and the 3 target analytes for which the ORNL practical holding times were exceeded are listed in Table 4-4. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables. Data in Tables 4-3 and 4-4 should not be considered quantitative and may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

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, 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 1995b). Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the 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.

Both PNL and ORNL report target analyte concentrations in ppmv of analyte in dry air. The results given may be corrected for the measured water vapor content of tank T-111 to obtain concentration in ppmv of analyte in moist tank air by multiplying the dry-air ppmv concentrations by 0.985.

Ten 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. Results from these 2 sampling and analytical methods are in good agreement for ethanenitrile, toluene, and n-decane. Four other compounds listed in Table 4-5 were determined by both laboratories to be below the 0.005 ppmv reporting limit of SUMMA™ samples. The remaining 3 compounds in Table 4-5 differ by less than a factor of 2.5, which must apparently be attributed to analytical inaccuracies. None of the discrepant compounds are at levels of concern.

The most abundant analytes in Tables 4-1 through 4-4 are n-tridecane and acetone. n-Tridecane, present in ORNL TSTs at about 1.1 ppmv, is the only compound observed above 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 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 (i.e., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (i.e., butanal) from SUMMATM 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 tentatively identified compounds detected in TST samples, and their estimated concentrations, are listed 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 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. 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 particularly long and difficult to analyze, the list has been sorted alphanumerically by compound name in Table 4-8. Table 4-9 gives the same list, sorted in order of decreasing estimated concentration. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the location of the compound in Table 4-7.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Klinger et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 through 4-9 should be considered rough estimates. Results in Tables 4-6 through 4-9 are presented in terms of observed chromatographic peaks, and are not adjusted for the occurrence of split peaks or the assignment of the same identity to different peaks (e.g., Cmpd # 48 and 49 in Table 4-7). In these instances, the estimated concentration of a compound appearing in more than 1 peak is simply the sum of the individual peak estimates.

4.3 Discussion of Organic Compounds

The organic compounds listed in Tables 4-1 through 4-9 may be classified as either 1) organic compounds added to tank T-111 as waste that are still evaporating, or 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 tentatively identified decahydronaphthalenes, alkyl-substituted cyclic, semivolatile branched, and semivolatile straight-chain alkanes. These 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 distribution of the NPHs in tank T-111 headspace suggests that significant preferential evaporation of the lighter species has occurred, making the n-tridecane and n-tetradecane the dominant species.

Many of the semivolatile alkanes found in tank T-111 are cyclic or branched. Examination of Table 4-8 indicates many alkyl-substituted cyclohexanes, hydrogenated and methylated naphthalenes, and branched alkanes. These are also prominent in Table 4-9, where the tentatively identified organic compounds in TST samples have been ranked by their estimated concentrations. By contrast, there are other 241-C farm tanks, notably tank C-102 (Huckaby 1995), in which the semivolatile alkane character is heavily dominated by the NPHs.

Though tributyl phosphate was not directly detected in the tank T-111 samples, its existence in the waste (probably at trace levels) can be inferred from the existence of the NPHs and 1-butanol. The 1-butanol detected in ORNL TST samples is a product of the hydrolysis of tributyl phosphate, and is virtually always detected when the NPHs are present.

Halogenated compounds, such as dichloromethane, trichloromethane, and tetrachloroethene may also have been placed into the waste tanks as cleaning solvent waste. These are denser than water, and may be present in small pools under the aqueous wastes. The origin of trichlorofluoromethane is unknown, but may be associated with urethane foams used to seal pit covers to reduce fugitive emissions. This particular compound is commonly detected as headspace constituents by both TST and SUMMA™ sample analyses.

The tentatively identified cyclosiloxane (i.e., Cmpd # 6 in Table 4-6 and Cmpd # 15 in Table 4-7) may also be in this category. Small quantities of siloxanes may have been introduced to the waste tank through their use as process surfactants or the disposal of contaminated hydraulic fluids. They may also be present in the headspace due to their use in liquid traps at the tank's breather riser. These compounds are frequently detected at very low levels in blanks, so it is also possible these are laboratory or sampling contaminants.

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

Ambient air SUMMA™ samples collected at the start of the tank T-111 sampling event indicate ethanenitrile, trimethylsilanol, and hexamethylsiloxane were present at trace levels in the sample collected via the heated VSS manifold. Of these, only the ethanenitrile was detected in the sample of the atmosphere upwind of tank T-111. Because these compounds were at much higher concentrations in the tank headspace than in the ambient air, their presence in the ambient air is thought to have a negligible effect on tank T-111.

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. However, the measured ammonia concentration of 226 ppmv does exceed the industrial hygiene notification limit of 150 ppmv. It was determined that no other headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Horn 1995).

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Table 2-1
Tank T-111 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 T-111 Inorganic Gas and Vapor Concentrations –
Analyses by Pacific Northwest Laboratory

Compound	CAS ¹ Number	Sample Type	Number of Samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	226	1	0.4
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	68.6	5	7
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	—	—
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 94	—	—
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.06	—	—
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.09	—	—
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	< 12.6	—	—
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	15,700 (11.8 mg/L)	300 (0.2 mg/L)	1.6

1 CAS = Chemical Abstracts Service.

2 RSD = relative standard deviation.

Table 4-1
Tank T-111 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation ³ (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.051	0.008	16
2	Propanone (acetone)	67-64-1	0.16	0.02	13
3	Trichlorofluoromethane	75-69-4	0.005	0.0004	8
4	Dichloromethane (methylene chloride)	75-09-2	0.008	0.001	11
5	Propanenitrile	107-12-0	0.009	0.002	20
6	1-Propanol ⁵	71-23-8	0.007	—	—
7	2-Butanone	78-93-3	0.015	0.0005	3
8	Trichloromethane (chloroform)	67-66-3	0.010	0.002	18
9	Pyridine ⁶	110-86-1	0.013	0.008	—
10	Toluene	108-88-3	0.012	0.001	6
11	Tetrachloroethene (tetrachloroethylene)	127-18-4	0.014	0.001	7
12 & 13	para-Xylene and meta-Xylene ⁷	106-42-3 108-38-3	0.006	0.0003	5
14	n-Decane	124-18-5	0.027	0.001	5
15	Methane	74-82-8	< 61	—	—

1 CAS = Chemical Abstract Service.

2 Average of 3 samples.

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

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

5 Detected in only one sample.

6 Detected in only two samples.

7 m-xylene and p-xylene coelute and the reported value represents the sum of their concentrations.

Table 4-2
Tank T-111 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	0.057	0.026	46
2	Propanone (acetone)	67-64-1	0.073	0.009	12
3	Toluene	108-88-3	0.015	0.0008	5
4	2-Hexanone	591-78-6	0.0069	0.0012	18
5	n-Hexanenitrile	628-73-9	0.0049	0.0007	14
6	2-Heptanone	110-43-0	0.0090	0.0022	24
7	n-Nonane	111-84-2	0.015	0.001	6
8	n-Heptanenitrile	629-08-3	0.0042	0.0009	21
9	2-Octanone	111-13-7	0.0048	0.0021	43
10	n-Decane	124-18-5	0.024	0.002	9
11	n-Undecane	1120-21-4	0.013	0.002	14

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

Table 4-3
Tank T-111 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	0.0033	0.0030	92
2	Propanenitrile	107-12-0	0.0042	0.0005	12
3	n-Hexane	110-54-3	0.0014	0.0002	13
4	Benzene	71-43-2	0.0046	0.0011	24
5	n-Butanenitrile	109-74-0	0.0055	0.0004	8
6	n-Heptane	142-82-5	0.0013	0.0003	20
7	n-Pentanenitrile	110-59-8	0.0034	0.00005	2
8	n-Octane	111-65-9	0.00094	0.00004	4
9	n-Dodecane	112-40-3	0.19	0.02	11
10	n-Tridecane	629-50-5	1.1	0.2	14

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 TST samples.

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

Table 4-4

**Tank T-111 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	0.0027	0.0005	20
2	1-Butanol ⁵	71-36-3	0.0058	0.0005	9
3	2-Pentanone ⁶	107-87-9	0.0082	0.0015	18

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

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

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

Table 4-5
Tank T-111 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Oak Ridge National Laboratory
and Pacific Northwest 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	0.0033	0.008	83
Propanone (acetone)	67-64-1	0.073	0.16	75
Ethanenitrile (acetonitrile)	75-05-8	0.057	0.051	11
Propanenitrile	107-12-0	0.0042	0.009	73
n-Butanenitrile	109-74-0	0.0055	< 0.005	> 10
Benzene	71-43-2	0.0046	< 0.005	—
Toluene	108-88-3	0.015	0.012	22
n-Hexane	110-54-3	0.0014	< 0.005	—
n-Heptane	142-82-5	0.0013	< 0.005	—
n-Decane	124-18-5	0.024	0.027	12

1 CAS = Chemical Abstract Service.

2 Average of 3, 1-L TST samples analyses.

3 Average of 3 sample analyses.

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

Table 4-6
Tank T-111 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation ³ (mg/m ³)
1	Ethanal (acetaldehyde)	75-07-0	< 0.02	--
2	Methanol (methyl alcohol)	67-56-1	0.35	0.04
3	Silanol, trimethyl-	1066-40-6	< 0.04	--
4	Butanal ⁴	123-72-8	0.11	--
5	2-Pentanone	107-87-9	0.06	0.01
6	Cyclotrisiloxane, hexamethyl-	541-05-9	< 0.10	--
7	2-Propanol, 2-methyl- ⁴	75-65-0	0.06	--
8	Unknown C8 Ketone		0.11	0.01
9	Unknown C9 Alkene/Cycloalkane		< 0.06	--
10	Decane, 4-methyl-	2847-72-5	0.09	0.005
11	Cyclohexane, butyl- ⁵	1678-93-9	0.07	0.005
12	n-Undecane	1120-21-4	0.10	0.01
13	n-Dodecane	112-40-3	2.94	0.26
14	Unknown Alkane		0.05	0.005
15	n-Tridecane	629-50-5	10.85	0.55
16	n-Tetradecane	629-59-4	6.00	0.44

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 samples, presented values 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 T-111 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	Carbon Dioxide	124-38-9	0.15	0.27
2	Carbon Dioxide	124-38-9	0.057	0.099
3	Carbon Dioxide	124-38-9	0.68	1.18
4	Methyl Alcohol	67-56-1	0.072	0.062
5	Trichloromonofluoro-methane	75-69-4	0.040	0.055
6	Silane, chlorotrimethyl-	75-77-4	0.0049	0.0085
7	Isopropyl Alcohol	67-63-0	0.0084	0.0073
8	2-Butanone	78-93-3	0.011	0.010
9	1-Pentene, 2,4,4-trimethyl-	107-39-1	0.019	0.004
10	Methyl Isobutyl Ketone	108-10-1	0.010	0.009
11	1-Pentanol	71-41-0	0.0061	0.0055
12	2-Pentanone, 4,4-dimethyl	590-50-1	0.0069	0.0061
13	Hexanal	66-25-1	0.0060	0.0054
14	Tetrachloroethylene	127-18-4	0.12	0.02
15	Cyclotrisiloxane, hexamethyl	541-05-9	0.041	0.036
16	Alkyl ester of nitric acid and others		0.0035	0.0060
17	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.035	0.027
18	Cyclohexane, 1,2,4- trimethyl- (1.alpha., 2.beta., 4.beta.)-	7667-60-9	0.014	0.002
19	C2-benzene		0.0038	0.0066
20	Cyclopentane, 1,2- dimethyl-, trans-	822-50-4	0.021	0.002
21	Benzene, 1,3-dimethyl-	108-38-3	0.049	0.001
22	Cyclohexane, 1,1,2-trimethyl-	7094-26-0	0.022	0.004
23	Cyclohexane, 1-ethyl- 4-methyl-, cis-	4926-78-7	0.014	0.004
24	3-Decene	19398-37-9	0.022	0.004
25	Cyclohexane, 1,1,3,5- tetramethyl-, cis-	50876-32-9	0.012	0.003

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
26	Cyclohexane, 1-ethyl- 4-methyl-, cis-	4926-78-7	0.020	0.003
27	Cyclohexanone, 3-methyl-	591-24-2	0.021	0.003
28	Octane, 2,5-dimethyl-	15869-89-3	0.014	0.002
29	Bicyclo[3.3.1]nonane	280-65-9	0.047	0.005
30	Octane, 2,6-dimethyl-	2051-30-1	0.048	0.003
31	Cyclohexane, propyl	1678-92-8	0.069	0.011
32	1-Decene	872-05-9	0.018	0.002
33	4-Nonene, 2,3,3-trimethyl-, (Z)	63830-68-2	0.0065	0.0113
34	Cyclohexane, 1,1,3,5- tetramethyl-, cis-	50876-32-9	0.011	0.020
35	Heptane, 3-ethyl-	15869-80-4	0.038	0.006
36	2-Heptanone, 6-methyl	928-68-7	0.069	0.043
37	Nonane, 4-methyl-	17301-94-9	0.037	0.001
38	Nonane, 2-methyl-	871-83-0	0.035	0.005
39	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.088	0.014
40	Nonane, 3-methyl-	5911-04-6	0.054	0.005
41	Benzene, 1,3,5-trimethyl-	108-67-8	0.020	0.009
42	1-Methyl-4-(1-methyl- ethyl)-cyclohexane	99-82-1	0.023	0.002
43	Cyclotetrasiloxane, octamethyl	556-67-2	0.050	0.044
44	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.057	0.009
45	1,2,4-Trimethyl- benzene	95-63-6	0.030	0.006
46	Cyclohexane, 1-methyl-2-propyl	4291-79-6	0.021	0.001
47	3-Heptene, 2,2,3,5,5, 6,6-heptamethyl-	54845-26-0	0.047	0.009
48	Decane, 4-methyl-	2847-72-5	0.078	0.013
49	Decane, 4-methyl-	2847-72-5	0.0063	0.0110
50	Undecane, 4-methyl-	2980-69-0	0.0059	0.0103
51	1-Hexanol, 2-ethyl-	104-76-7	0.077	0.036
52	Decane, 2,9-dimethyl- and others		0.014	0.003

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
53	Cyclohexane, butyl-	1678-93-9	0.044	0.006
54	alkane and others		0.030	0.026
55	alkanal		0.019	0.017
56	Decane, 5-methyl-	13151-35-4	0.011	0.001
57	5-Undecene	4941-53-1	0.038	0.001
58	Decane, 2-methyl-	6975-98-0	0.0069	0.0060
59	Undecanal, 2-methyl- and c4-benzene		0.026	0.023
60	Decane, 3-methyl-	13151-34-3	0.011	0.002
61	Naphthalene, decahydro-, trans-	493-02-7	0.031	0.004
62	Benzene, (1-methylpropyl)-	135-98-8	0.020	0.003
63	Octanenitrile and others		0.014	0.002
64	3-Undecene, (E)-	1002-68-2	0.0078	0.0134
65	Cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.011	0.010
66	2-Nonanone	821-55-6	0.017	0.015
67	Cyclohexane, 1-ethyl- 4-methyl-, trans	6236-88-0	0.0040	0.0069
68	Nonanal	124-19-6	0.018	0.017
69	Benzene, (1,1-dimethylpropyl)-	2049-95-8	0.013	0.011
70	Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	0.0096	0.0085
71	Undecane, 4-methyl-	2980-69-0	0.0044	0.0080
72	Carbon dioxide and others		0.0061	0.0106
73	Carbon dioxide and others		0.044	0.076
74	Undecane, 2,8- dimethyl and others		0.0062	0.0107
75	3-Ethyl-2-methyl-2- pentanol and alkyl benzene		0.031	0.006
76	5-Decanone	820-29-1	0.028	0.025
77	3-Octanol, 3,7-dimethyl-, (+/-)-	57706-88-4	0.0059	0.0054
78	n-Amylcyclohexane	4292-92-6	0.010	0.002
79	Naphthalene, decahydro-2-methyl-	2958-76-1	0.012	0.003

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
80	2-Undecanone and alkyl benzene		0.031	0.009
81	Benzene, (1-cyclohexylethyl)- and others		0.021	0.002
82	Benzene, pentyl- and others		0.018	0.004
83	1-Nonanol	143-08-8	0.014	0.002
84	5-Undecanone, 2-methyl-	50639-02-6	0.012	0.011
85	3-Pentanol, 2,3,4-trimethyl-	3054-92-0	0.0067	0.0060
86	Cyclooctanemethanol, .alpha.,.alpha.-dimethyl-	16624-06-9	0.018	0.002
87	3-Decanone and alkyl benzene		0.034	0.011
88	2-Decanone	693-54-9	0.023	0.020
89	alkyl-cyclohexane		0.012	0.004
90	Naphthalene and others		0.081	0.009
91	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.025	0.004
92	Cyclohexane, hexyl	4292-75-5	0.030	0.004
93	Undecane, 4,8-dimethyl-	17301-33-6	0.020	0.005
94	Dodecane, 2-methyl-6-propyl-	55045-08-4	0.024	0.005
95	Tridecane, 7-methyl-	26730-14-3	0.097	0.013
96	Trimethyl-decahydro-naphthalene		0.0085	0.0078
97	1-Octanol, 2-butyl	3913-02-8	0.025	0.044
98	3-Undecanone	2216-87-7	0.0081	0.0073
99	Dodecane, 2,5-dimethyl-	56292-65-0	0.043	0.015
100	Naphthalene, 2-methyl-	91-57-6	0.026	0.003
101	Tetradecane	629-59-4	0.048	0.0062
102	C7-Cyclohexane		0.064	0.010
103	Tridecane, 2-methyl-	1560-96-9	0.035	0.005
104	Tetradecane, 4-methyl	25117-24-2	0.035	0.003
105	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.14	0.02
106	Ethanone,1-(2,4,5-trimethylphenyl)-	2040-07-5	0.011	0.010
107	Cyclotetradecane and others		0.0090	0.0157

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
108	7-Tetradecene	10374-74-0	0.019	0.009
109	Tetradecane	629-59-4	7.65	1.08
110	Diphenyl ether	101-84-8	0.18	0.02
111	Naphthalene, 2,3-dimethyl-	581-40-8	0.0039	0.0067
112	Naphthalene, 1,7-dimethyl-	575-37-1	0.0074	0.0074
113	2,7-Dimethyl-2,7-octanediol	19781-07-8	0.014	0.013
114	Hexadecane	544-76-3	0.083	0.015
115	6-Tridecanone	22026-12-6	0.031	0.011
116	Tridecanol	26248-42-0	0.0032	0.0056
117	3-Tridecanone	1534-26-5	0.013	0.0116
118	Pentadecane	629-62-9	0.44	0.07
119	6-Tridecanone	22026-12-6	0.013	0.003
120	Hexadecane	544-76-3	0.028	0.005
121	2-Tetradecanone	2345-27-9	0.0075	0.0074
122	alkenol		0.014	0.006
123	Benzenesulfonamide, N-butyl	3622-84-2	0.021	0.0114
124	Isopropyl Palmitate	142-91-6	0.017	0.020
Sum of tentatively identified compounds:			12.4	

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 samples, presented values are estimates.

Table 4-8
Tank T-111 Tentatively Identified Organic Compounds in TST Samples
in Alphanumerical Order --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	alkanal		0.019	0.017
54	alkane and others		0.030	0.026
122	alkenol		0.014	0.006
89	alkyl-cyclohexane		0.012	0.004
16	Alkyl ester of nitric acid and others		0.0035	0.0060
69	Benzene, (1,1-dimethylpropyl)-	2049-95-8	0.013	0.011
62	Benzene, (1-methylpropyl)-	135-98-8	0.020	0.003
41	Benzene, 1,3,5-trimethyl-	108-67-8	0.020	0.009
81	Benzene, (1-cyclohexylethyl)- and others		0.021	0.002
70	Benzene, 1-methyl- 3-(1-methylethyl)-	535-77-3	0.0096	0.0085
82	Benzene, pentyl- and others		0.018	0.004
21	Benzene, 1,3-dimethyl-	108-38-3	0.049	0.001
123	Benzenesulfonamide, N-butyl	3622-84-2	0.021	0.0114
1	Carbon Dioxide	124-38-9	0.15	0.27
3	Carbon Dioxide	124-38-9	0.68	1.18
2	Carbon Dioxide	124-38-9	0.057	0.099
72	Carbon dioxide and others		0.0061	0.0106
73	Carbon dioxide and others		0.044	0.076
39	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.088	0.014
26	Cyclohexane, 1-ethyl- 4-methyl-, cis-	4926-78-7	0.020	0.003
67	Cyclohexane, 1-ethyl- 4-methyl-, trans	6236-88-0	0.0040	0.0069
23	Cyclohexane, 1-ethyl- 4-methyl-, cis-	4926-78-7	0.014	0.004
18	Cyclohexane, 1,2,4- trimethyl- (1.alpha., 2.beta., 4.beta.)-	7667-60-9	0.014	0.002
46	Cyclohexane, 1-methyl-2-propyl	4291-79-6	0.021	0.001
44	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.057	0.009

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
65	Cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.011	0.010
17	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.035	0.027
22	Cyclohexane, 1,1,2-trimethyl-	7094-26-0	0.022	0.004
92	Cyclohexane, hexyl	4292-75-5	0.030	0.004
31	Cyclohexane, propyl	1678-92-8	0.069	0.011
25	Cyclohexane, 1,1,3,5- tetramethyl-, cis-	50876-32-9	0.012	0.003
34	Cyclohexane, 1,1,3,5- tetramethyl-, cis-	50876-32-9	0.011	0.020
53	Cyclohexane, butyl-	1678-93-9	0.044	0.006
91	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.025	0.004
27	Cyclohexanone, 3-methyl-	591-24-2	0.021	0.003
86	Cyclooctanemethanol, .alpha.,.alpha.-dimethyl-	16624-06-9	0.018	0.002
20	Cyclopentane, 1,2- dimethyl-, trans-	822-50-4	0.021	0.002
107	Cyclotetradecane and others		0.0090	0.0157
43	Cyclotetrasiloxane, octamethyl	556-67-2	0.050	0.044
15	Cyclotrisiloxane, hexamethyl	541-05-9	0.041	0.036
52	Decane, 2,9-dimethyl- and others		0.014	0.003
48	Decane, 4-methyl-	2847-72-5	0.078	0.013
60	Decane, 3-methyl-	13151-34-3	0.011	0.002
58	Decane, 2-methyl-	6975-98-0	0.0069	0.0060
49	Decane, 4-methyl-	2847-72-5	0.0063	0.0110
56	Decane, 5-methyl-	13151-35-4	0.011	0.001
110	Diphenyl ether	101-84-8	0.18	0.02
105	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.14	0.02
99	Dodecane, 2,5-dimethyl-	56292-65-0	0.043	0.015
94	Dodecane, 2-methyl-6-propyl-	55045-08-4	0.024	0.005
106	Ethanone, 1-(2,4,5-trimethylphenyl)-	2040-07-5	0.011	0.010
35	Heptane, 3-ethyl-	15869-80-4	0.038	0.006
114	Hexadecane	544-76-3	0.083	0.015

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
120	Hexadecane	544-76-3	0.028	0.005
13	Hexanal	66-25-1	0.0060	0.0054
124	Isopropyl Palmitate	142-91-6	0.017	0.020
7	Isopropyl Alcohol	67-63-0	0.0084	0.0073
10	Methyl Isobutyl Ketone	108-10-1	0.010	0.009
4	Methyl Alcohol	67-56-1	0.072	0.062
78	n-Amylcyclohexane	4292-92-6	0.010	0.002
61	Naphthalene, decahydro-, trans-	493-02-7	0.031	0.004
90	Naphthalene and others		0.081	0.009
79	Naphthalene, decahydro-2-methyl-	2958-76-1	0.012	0.003
100	Naphthalene, 2-methyl-	91-57-6	0.026	0.003
111	Naphthalene, 2,3-dimethyl-	581-40-8	0.0039	0.0067
112	Naphthalene, 1,7-dimethyl-	575-37-1	0.0074	0.0074
68	Nonanal	124-19-6	0.018	0.017
38	Nonane, 2-methyl-	871-83-0	0.035	0.005
37	Nonane, 4-methyl-	17301-94-9	0.037	0.001
40	Nonane, 3-methyl-	5911-04-6	0.054	0.005
28	Octane, 2,5-dimethyl-	15869-89-3	0.014	0.002
30	Octane, 2,6-dimethyl-	2051-30-1	0.048	0.003
63	Octanenitrile and others		0.014	0.002
118	Pentadecane	629-62-9	0.44	0.07
6	Silane, chlorotrimethyl-	75-77-4	0.0049	0.0085
14	Tetrachloroethylene	127-18-4	0.12	0.02
104	Tetradecane, 4-methyl	25117-24-2	0.035	0.003
109	Tetradecane	629-59-4	7.65	1.08
101	Tetradecane	629-59-4	0.048	0.0062
5	Trichloromonofluoro-methane	75-69-4	0.040	0.055
95	Tridecane, 7-methyl-	26730-14-3	0.097	0.013
103	Tridecane, 2-methyl-	1560-96-9	0.035	0.005

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
116	Tridecanol	26248-42-0	0.0032	0.0056
96	Trimethyl-decahydro-naphthalene		0.0085	0.0078
59	Undecanal, 2-methyl- and c4-benzene		0.026	0.023
50	Undecane, 4-methyl-	2980-69-0	0.0059	0.0103
71	Undecane, 4-methyl-	2980-69-0	0.0044	0.0080
93	Undecane, 4,8-dimethyl-	17301-33-6	0.020	0.005
74	Undecane, 2,8- dimethyl and others		0.0062	0.0107
42	1-Methyl-4-(1-methylethyl)- cyclohexane	99-82-1	0.023	0.002
9	1-Pentene, 2,4,4-trimethyl-	107-39-1	0.019	0.004
83	1-Nonanol	143-08-8	0.014	0.002
11	1-Pentanol	71-41-0	0.0061	0.0055
51	1-Hexanol, 2-ethyl-	104-76-7	0.077	0.036
32	1-Decene	872-05-9	0.018	0.002
97	1-Octanol, 2-butyl	3913-02-8	0.025	0.044
66	2-Nonanone	821-55-6	0.017	0.015
36	2-Heptanone, 6-methyl	928-68-7	0.069	0.043
8	2-Butanone	78-93-3	0.011	0.010
12	2-Pentanone, 4,4-dimethyl	590-50-1	0.0069	0.0061
88	2-Decanone	693-54-9	0.023	0.020
121	2-Tetradecanone	2345-27-9	0.0075	0.0074
80	2-Undecanone and alkyl benzene		0.031	0.009
19	C2-benzene		0.0038	0.0066
117	3-Tridecanone	1534-26-5	0.013	0.0116
85	3-Pentanol, 2,3,4-trimethyl-	3054-92-0	0.0067	0.0060
98	3-Undecanone	2216-87-7	0.0081	0.0073
47	3-Heptene, 2,2,3,5,5,6,6-heptamethyl-	54845-26-0	0.047	0.009
24	3-Decene	19398-37-9	0.022	0.004
75	3-Ethyl-2-methyl-2- pentanol and alkyl benzene		0.031	0.006

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
64	3-Undecene, (E)-	1002-68-2	0.0078	0.0134
87	3-Decanone and alkyl benzene		0.034	0.011
77	3-Octanol, 3,7-dimethyl-, (+/-)-	57706-88-4	0.0059	0.0054
29	Bicyclo[3.3.1]nonane	280-65-9	0.047	0.005
33	4-Nonene, 2,3,3-trimethyl-, (Z)	63830-68-2	0.0065	0.0113
84	5-Undecanone, 2-methyl-	50639-02-6	0.012	0.011
76	5-Decanone	820-29-1	0.028	0.025
57	5-Undecene	4941-53-1	0.038	0.001
119	6-Tridecanone	22026-12-6	0.013	0.003
115	6-Tridecanone	22026-12-6	0.031	0.011
108	7-Tetradecene	10374-74-0	0.019	0.009
102	C7-Cyclohexane		0.064	0.010
113	2,7-Dimethyl-2,7-octanediol	19781-07-8	0.014	0.013
45	1,2,4-Trimethylbenzene	95-63-6	0.030	0.006

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 samples, presented values are estimates.

Table 4-9
Tank T-111 Tentatively Identified Organic Compounds in TST Samples
in Order of Estimated Concentrations –
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
109	Tetradecane	629-59-4	7.65	1.08
3	Carbon Dioxide	124-38-9	0.68	1.18
118	Pentadecane	629-62-9	0.44	0.07
110	Diphenyl ether	101-84-8	0.18	0.02
1	Carbon Dioxide	124-38-9	0.15	0.27
105	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.14	0.02
14	Tetrachloroethylene	127-18-4	0.12	0.02
95	Tridecane, 7-methyl-	26730-14-3	0.097	0.013
39	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.088	0.014
114	Hexadecane	544-76-3	0.083	0.015
90	Naphthalene and others		0.081	0.009
48	Decane, 4-methyl-	2847-72-5	0.078	0.013
51	1-Hexanol, 2-ethyl-	104-76-7	0.077	0.036
4	Methyl Alcohol	67-56-1	0.072	0.062
31	Cyclohexane, propyl	1678-92-8	0.069	0.011
36	2-Heptanone, 6-methyl	928-68-7	0.069	0.043
102	C7-Cyclohexane		0.064	0.010
2	Carbon Dioxide	124-38-9	0.057	0.099
44	Cyclohexane, 1-methyl-2-propyl-	4291-79-6	0.057	0.009
40	Nonane, 3-methyl-	5911-04-6	0.054	0.005
43	Cyclotetrasiloxane, octamethyl	556-67-2	0.050	0.044
21	Benzene, 1,3-dimethyl-	108-38-3	0.049	0.001
101	Tetradecane	629-59-4	0.048	0.0062
30	Octane, 2,6-dimethyl-	2051-30-1	0.048	0.003
29	Bicyclo[3.3.1]nonane	280-65-9	0.047	0.005
47	3-Heptene, 2,2,3,5,5, 6,6-heptamethyl-	54845-26-0	0.047	0.009
73	Carbon dioxide and others		0.044	0.076

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
53	Cyclohexane, butyl-	1678-93-9	0.044	0.006
99	Dodecane, 2,5-dimethyl-	56292-65-0	0.043	0.015
15	Cyclotrisiloxane, hexamethyl	541-05-9	0.041	0.036
5	Trichloromonofluoro-methane	75-69-4	0.040	0.055
57	5-Undecene	4941-53-1	0.038	0.001
35	Heptane, 3-ethyl-	15869-80-4	0.038	0.006
37	Nonane, 4-methyl-	17301-94-9	0.037	0.001
104	Tetradecane, 4-methyl	25117-24-2	0.035	0.003
17	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.035	0.027
103	Tridecane, 2-methyl-	1560-96-9	0.035	0.005
38	Nonane, 2-methyl-	871-83-0	0.035	0.005
87	3-Decanone and alkyl benzene		0.034	0.011
115	6-Tridecanone	22026-12-6	0.031	0.011
61	Naphthalene, decahydro-, trans-	493-02-7	0.031	0.004
80	2-Undecanone and alkyl benzene		0.031	0.009
75	3-Ethyl-2-methyl-2-pentanol and alkyl benzene		0.031	0.006
54	alkane and others		0.030	0.026
45	1,2,4-Trimethyl-benzene	95-63-6	0.030	0.006
92	Cyclohexane, hexyl	4292-75-5	0.030	0.004
76	5-Decanone	820-29-1	0.028	0.025
120	Hexadecane	544-76-3	0.028	0.005
59	Undecanal, 2-methyl- and c4-benzene		0.026	0.023
100	Naphthalene, 2-methyl-	91-57-6	0.026	0.003
97	1-Octanol, 2-butyl	3913-02-8	0.025	0.044
91	Cyclohexane, 2-butyl- 1,1,3-trimethyl-	54676-39-0	0.025	0.004
94	Dodecane, 2-methyl-6-propyl-	55045-08-4	0.024	0.005
88	2-Decanone	693-54-9	0.023	0.020

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
42	1-Methyl-4-(1-methyl-ethyl)-cyclohexane	99-82-1	0.023	0.002
24	3-Decene	19398-37-9	0.022	0.004
22	Cyclohexane, 1,1,2-trimethyl-	7094-26-0	0.022	0.004
27	Cyclohexanone, 3-methyl-	591-24-2	0.021	0.003
46	Cyclohexane, 1-methyl-2-propyl	4291-79-6	0.021	0.001
20	Cyclopentane, 1,2- dimethyl-, trans-	822-50-4	0.021	0.002
123	Benzenesulfonamide, N-butyl	3622-84-2	0.021	0.0114
81	Benzene, (1-cyclohexylethyl)- and others		0.021	0.002
62	Benzene, (1-methylpropyl)-	135-98-8	0.020	0.003
41	Benzene, 1,3,5-trimethyl-	108-67-8	0.020	0.009
26	Cyclohexane, 1-ethyl- 4-methyl-, cis-	4926-78-7	0.020	0.003
93	Undecane, 4,8-dimethyl-	17301-33-6	0.020	0.005
55	alkanal		0.019	0.017
108	7-Tetradecene	10374-74-0	0.019	0.009
9	1-Pentene, 2,4,4-trimethyl-	107-39-1	0.019	0.004
68	Nonanal	124-19-6	0.018	0.017
82	Benzene, pentyl- and others		0.018	0.004
32	1-Decene	872-05-9	0.018	0.002
86	Cyclooctanemethanol, .alpha.,.alpha.-dimethyl-	16624-06-9	0.018	0.002
124	Isopropyl Palmitate	142-91-6	0.017	0.020
66	2-Nonanone	821-55-6	0.017	0.015
23	Cyclohexane, 1-ethyl- 4-methyl-, cis-	4926-78-7	0.014	0.004
113	2,7-Dimethyl-2,7-octanediol	19781-07-8	0.014	0.013
122	alkenol		0.014	0.006
28	Octane, 2,5-dimethyl-	15869-89-3	0.014	0.002
52	Decane, 2,9-dimethyl- and others		0.014	0.003
63	Octanenitrile and others		0.014	0.002

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
18	Cyclohexane, 1,2,4- trimethyl- (1.alpha., 2.beta.,4.beta.)-	7667-60-9	0.014	0.002
83	1-Nonanol	143-08-8	0.014	0.002
119	6-Tridecanone	22026-12-6	0.013	0.003
117	3-Tridecanone	1534-26-5	0.013	0.0116
69	Benzene, (1,1-dimethylpropyl)-	2049-95-8	0.013	0.011
84	5-Undecanone, 2-methyl-	50639-02-6	0.012	0.011
25	Cyclohexane, 1,1,3,5- tetramethyl-, cis-	50876-32-9	0.012	0.003
89	alkyl-cyclohexane		0.012	0.004
79	Naphthalene, decahydro-2-methyl-	2958-76-1	0.012	0.003
60	Decane, 3-methyl-	13151-34-3	0.011	0.002
56	Decane, 5-methyl-	13151-35-4	0.011	0.001
65	Cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.011	0.010
8	2-Butanone	78-93-3	0.011	0.010
106	Ethanone, 1-(2,4,5- trimethylphenyl)-	2040-07-5	0.011	0.010
34	Cyclohexane, 1,1,3,5- tetramethyl-, cis-	50876-32-9	0.011	0.020
10	Methyl Isobutyl Ketone	108-10-1	0.010	0.009
78	n-Amylcyclohexane	4292-92-6	0.010	0.002
70	Benzene, 1-methyl- 3-(1-methylethyl)-	535-77-3	0.0096	0.0085
107	Cyclotetradecane and others		0.0090	0.0157
96	Trimethyl-decahydro-naphthalene		0.0085	0.0078
7	Isopropyl Alcohol	67-63-0	0.0084	0.0073
98	3-Undecanone	2216-87-7	0.0081	0.0073
64	3-Undecene, (E)-	1002-68-2	0.0078	0.0134
121	2-Tetradecanone	2345-27-9	0.0075	0.0074
112	Naphthalene, 1,7-dimethyl-	575-37-1	0.0074	0.0074
58	Decane, 2-methyl-	6975-98-0	0.0069	0.0060
12	2-Pentanone, 4,4-dimethyl	590-50-1	0.0069	0.0061

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
85	3-Pentanol, 2,3,4-trimethyl-	3054-92-0	0.0067	0.0060
33	4-Nonene, 2,3,3-trimethyl-, (Z)	63830-68-2	0.0065	0.0113
49	Decane, 4-methyl-	2847-72-5	0.0063	0.0110
74	Undecane, 2,8- dimethyl and others		0.0062	0.0107
72	Carbon dioxide and others		0.0061	0.0106
11	1-Pentanol	71-41-0	0.0061	0.0055
13	Hexanal	66-25-1	0.0060	0.0054
77	3-Octanol, 3,7-dimethyl-, (+/-)-	57706-88-4	0.0059	0.0054
50	Undecane, 4-methyl-	2980-69-0	0.0059	0.0103
6	Silane, chlorotrimethyl-	75-77-4	0.0049	0.0085
71	Undecane, 4-methyl-	2980-69-0	0.0044	0.0080
67	Cyclohexane, 1-ethyl- 4-methyl-, trans	6236-88-0	0.0040	0.0069
111	Naphthalene, 2,3-dimethyl-	581-40-8	0.0039	0.0067
19	C2-benzene		0.0038	0.0066
16	Alkyl ester of nitric acid and others		0.0035	0.0060
116	Tridecanol	26248-42-0	0.0032	0.0056

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 samples, presented values are estimates.

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