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TANK 241BY112 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
11/1994

ENGINEERING CHANGE NOTICE

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18. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 12. Enter the affected document number in Block 19.					
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Functional Design Criteria	☐	Stress/Design Report	☐	Health Physics Procedure	☐
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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	☐
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OM Manual	☐	Operational Safety Requirement	☐	ICRS Procedure	☐
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7. Abstract

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

8. RELEASE STAMP

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Tank 241-BY-112 Headspace Gas and Vapor Characterization Results for Samples Collected in November 1994

J. L. Huckaby
Pacific Northwest Laboratories

D. R. Bratzel
Westinghouse Hanford Company

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Westinghouse
Hanford Company

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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-BY-112 Headspace Gas and Vapor Characterization Results
for Samples Collected in November 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BY-112 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank BY-112 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994). Results presented here represent the best available data on the headspace constituents of tank BY-112.

1.2 Characterization Data Criteria

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

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank BY-112, 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 headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been representative of the tank BY-112 headspace when the tank was sampled, and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents (Meacham et al. 1995). No assessment has been made of how the tank BY-112 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in the passively ventilated tanks (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank BY-112 is the third tank in a 3-tank cascade with tanks BY-110 and BY-111. It is connected to tank BY-111 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade line. Tanks BY-110 and BY-111 are also connected by a similar line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank BY-110 or BY-111 may be transferred to tank BY-112 (unless the cascade lines are obstructed).

The cascade of tanks BY-110, BY-111, and BY-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 BY-112 using the vapor sampling system (VSS) on November 18, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-BY-112 Tank Characterization Plan* (Homi 1994). The tank headspace temperature was determined to be 23.3 °C. Air from the BY-112 headspace was withdrawn from a single elevation via a 7.9-m long heated sampling probe mounted in riser 21, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All tank air samples were collected between 11:06 a.m. and 2:26 p.m., with no anomalies noted.

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

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

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMATM¹ canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL, at PNL quality assurance impact level 2 (Clauss et al. 1995).

Analyses of the inorganic vapor sorbent traps were performed within 32 days of sample collection, and analyses of SUMMATM canisters for inorganic compounds were performed 88 days after sample collection (Ligotke 1995). Thus the administratively chosen 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994) was satisfied only for analyses of the sorbent traps. It should be noted that the inorganic compounds analyzed for in SUMMATM canisters would be expected to be very stable in the SUMMATM canisters, and the results may not have been affected even though the 60-day holding time requirement was exceeded.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in the headspace of tank BY-112 was measured at 63 ppmv. 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 63 ppmv corresponds to less than 0.05 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank BY-112 was determined to be < 94 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, 94 ppmv hydrogen concentration in tank BY-112 would correspond to about 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank BY-112.

The nitrous oxide concentration in tank BY-112 was measured at 40 ppmv. Nitrous oxide has been detected in other passively ventilated waste tanks at concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as about 868 ppmv in tank U-103 (Ligotke et al. 1995). Under proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank BY-112 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank BY-112 headspace was characterized as < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide has not been

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

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).

The average carbon dioxide concentration in the tank BY-112 headspace, 121 ppmv, is significantly lower than it is in ambient air. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient in the waste tank headspaces. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. The 121 ppmv of carbon dioxide measured in tank BY-112 is about average for the waste tanks sampled to date.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BY-112 headspace were determined to be 0.18 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank BY-112. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank BY-112 headspace.

The water vapor concentration of tank BY-112 was determined to be about 11.2 mg/L, at the measured tank headspace temperature of 23.3 °C and pressure of 1001 mbar (751 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 15.3 mbar (11.5 torr), to a dew point of 13.3 °C, and to a relative humidity of 53 %.

Silica gel sorbent traps were used to test 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 and carbon dioxide, the most abundant waste constituents in the tank BY-112 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces sampled to date, and along with hydrogen, are usually the dominate waste species.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are very good. Relative standard deviations range from 8.6 % for carbon dioxide to 15 % for nitrous oxide results. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), the small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

As discussed briefly in Section 1.4, it is possible that gases and vapors generated by the waste in tanks BY-110 and BY-111 could be transferred to tank BY-112 via the cascade lines. If significant exchange of selected inorganic gases and vapors were taking place between adjacent tanks, either their headspace

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

compositions would be very similar, or all constituents detected in one tank would be at or equal or higher concentrations in the other tank. The data in Table 3-2 are consistent with the premise that air, gases, and vapors could be transferring from tank BY-111 to tank BY-112 (waste species are at higher concentrations in tank BY-112 than in BY-111, and carbon dioxide is lower), but do not constitute proof that this is occurring.

4.0 ORGANIC VAPORS

Organic vapors in the tank BY-112 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatographs (GCs) equipped with mass spectrometer (MS) detectors were used by PNL and ORNL to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Clauss et al. (1995).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-112. These results were produced at PNL quality assurance impact level 2. However, PNL analyses were not completed until 81 days after sample collection, which was beyond the administratively chosen 60-day holding time of the WHC quality assurance project plan (Keller 1994). No holding time study has been done to determine the stability of organic analytes in SUMMA™ canisters in the chemical matrix of tank samples.

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

All TSTs prepared by ORNL had 3 surrogate compounds added to evaluate sample matrix effects, potential handling, storage, and shipment problems, and analytical instrumentation performance (Jenkins et al. 1995a). ORNL evaluated the surrogate recoveries using a statistical approach similar to that prescribed by *SW 846 Method 8260A Volatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS) Capillary Column Technique* (EPA 1992). Using this approach, ORNL reported that all surrogates had standard deviation values within the 95 % confidence interval for variance, indicating that no bias was introduced in the measurement of analyte quantities (Jenkins 1995a).

4.1 Positively Identified Organic Compounds

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

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list included the 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 tank C-103.

Table 4-1 lists the 4 organic compounds positively identified and quantitated in SUMMA™ samples. SUMMA™ organic analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Clauss et al. 1995). Only 2 of the 40 TO-14 target analytes and only 2 of the 14 additional target analytes were measured to be above the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

Jenkins et al. (1995a) report the positive identification of 24 of 27 target analytes in TST samples. 1,1-Dichloroethene, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected in the TST samples. The average concentrations of 3 quantitated target analytes, from the analysis of 3 TSTs, are given in Table 4-2. Table 4-3 lists 16 compounds which were determined to be outside of the instrument calibration range in at least 1 of the TST samples, and consequently not quantitated. The 5 other positively identified compounds are listed in Table 4-4 because analyses were performed after their ORNL analyte-specific practical holding times had been exceeded. Data in Tables 4-3 and 4-4 may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

Based on a practical holding time study performed by ORNL the reported concentrations of propanone, butanal, 1-butanol, 2-pentanone, and n-pentanenitrile may have been affected by the 62 day period between sample collection and analysis (Jenkins 1995b). The concentration of these five analytes are reported in Table 4-4. The practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. Jenkins et al. (1995b) describe the ORNL practical holding time study, and report practical holding times for these compounds.

Eleven target analytes were common to both TST and SUMMATM analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMATM samples. The data given in Table 4-5 indicate these methods agree that 8 of the 11 listed analytes are at or below about 0.006 ppmv. Propanone, ethanenitrile, and toluene are each reported to be at higher concentrations in TST samples than in SUMMATM samples.

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

4.2 Tentatively Identified Organic Compounds

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

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and 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 list of tentatively identified compounds recovered from SUMMATM samples, with estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table 4-7. Compounds are listed in Table 4-7 according to the order by which the eluted chromatographically. The

averages reported by ORNL in Table 4-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

Because the list of tentatively identified organic compounds in TST samples is long and locating any given compound may be difficult, the list has been sorted alphanumerically by compound name in Table 4-8, and also in order of decreasing estimated concentrations in Table 4-9. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the elution order of the compound in Table 4-7.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Clauss et al. (1995), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 through 4-9 should be considered rough estimates. Results in Tables 4-6 through 4-9 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 6 and 7 in Table 4-7) or the assignment of the same identity to different peaks (e.g., Cmpd # 53 and 58 in Table 4-7). In these instances, the estimated concentration of a compound appearing in different peaks is simply the sum of the individual peak estimates.

4.3 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-7 is to separate them into 2 categories: 1) Organic compounds added to tank BY-112 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

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

Trace amounts of a tentatively identified cyclosiloxane (i.e., Cmpd # 23 in Table 4-7) may also be in the category of waste additions. Small quantities of siloxanes may have been introduced to the waste tank through their use as process surfactants, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-9 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, alkyl nitrates, and volatile alkanes, all of which have been associated with the degradation of the NPHs. While both larger and smaller molecules are generated from the waste, the most abundant of these in the headspace are the smaller, short-chain volatile compounds.

Small amounts of the tributyl phosphate diluents and their degradation products is reason to expect trace amounts of tributyl phosphate to be present in the tank waste. The low volatility of tributyl phosphate, and its tendency to adsorb on glass fiber filters during sampling, apparently preclude its measurement in the tank BY-112 samples. 1-Butanol, known to be a product of the hydrolysis of tributyl phosphate, is at a relatively low concentration in the tank BY-112 samples. In TST samples, 1-butanol and other alcohols are at similar concentrations; the average methanol, ethanol, 2-propanol, and 1-butanol concentrations in TSTs samples are 0.36, 0.083, 0.13, and 0.20 mg/m³, respectively. Based on these considerations, it is likely that the amounts of tributyl phosphate in the tank BY-112 waste and headspace are very low.

The total organic vapor concentration of tank BY-112 was estimated by Jenkins et al. (1995a) to be about 5.8 mg/m³. This is the summation of concentrations of positively and tentatively identified compounds in 3 TST samples by GC/MS.

Tank BY-112 is known to have contained liquid tributyl phosphate "diluted with degraded kerosene" (Schulz 1968). Schulz's assessment of the organic liquid was in preparation for application of the In Tank Solidification (ITS) process to tank BY-112, and he states that "All, or, at least most, of the organic solution will likely steam distill during ITS operations in the 112 BY tank." The vapor samples collected in November 1994, seem to support Schulz' prediction. The total organic vapor concentration has been estimated to be relatively low, even compared to the other tanks to which it is connected (Table 3-2). Furthermore, the principle signature of tributyl phosphate in the headspace, 1-butanol, is also present at a relatively low concentration.

In summary, the tank BY-112 headspace has a moderate to low level of organic vapors. While having many of the same organic vapors as NPH-rich tanks, the alcohols are more prominent and the aldehydes less prevalent in tank BY-112. The organic liquid present in tank BY-112 before operation of the ITS process, while leaving its signature, apparently does not still exist.

5.0 SUMMARY

The tank BY-112 headspace was sampled in November 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).

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Table 2-1
Tank BY-112 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	0.1	Organic vapors	4 tank air samples
		0.5	Organic vapors	4 tank air samples
		2.0	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 BY-112 Inorganic Gas and Vapor Concentrations
Analyses Conducted 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	63	6	9.5
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	121	10	8.6
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	0.18	0.02	11
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	—	—
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	40	6	15
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	15,300 (11.2 mg/L)	1,300 (1.0 mg/L)	9

¹ CAS = Chemical Abstracts Service.

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

Table 3-2
Comparison of Tank BY-110, BY-111, and BY-112 Headspace Constituents¹

Tank:	BY-110 ²	BY-111 ³	BY-112
Date sampled, (mo/day/yr)	11/11/94	5/11/94 11/16/94	11/18/94
Headspace temperature, (°C)	27	27	23.2
Ammonia, (ppmv)	401	59	63
Hydrogen, (ppmv)	< 160	< 160	< 94
Carbon dioxide, (ppmv)	229	219	121
Carbon monoxide, (ppmv)	< 76	< 76	< 12
Nitric oxide, (ppmv)	≤ 0.09	≤ 0.15	0.18
Nitrogen dioxide, (ppmv)	≤ 0.05	≤ 0.05	≤ 0.02
Nitrous oxide, (ppmv)	103	< 67	40
Water vapor, (mg/m ³)	8.0	6.9	11.2
Water vapor, (% relative humidity)	31	27	53
Ethanenitrile (acetonitrile), (ppmv)	0.81	0.050	0.10
Propanone (acetone), (ppmv)	(3.8)	(0.48)	(1.0)
1-Butanol, (ppmv)	0.30	< 0.0011	0.059
n-Dodecane, (ppmv)	0.079	< 0.00046	0.0097
n-Tridecane, (ppmv)	0.13	(0.0015)	0.020
Total organic compounds ⁴ , (mg/m ³)	29	2.2	5.8

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

2 Data are from Huckaby and Bratzel 1995a.

3 Data are from Huckaby and Bratzel 1995b.

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

Table 4-1
Tank BY-112 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
1	Trichlorofluoromethane	75-69-4	0.21	0.02	10
2	Toluene	108-88-3	0.041	0.0004	1
3	2-Butanone	78-93-3	0.12	0.01	8
4	Propanone (acetone)	67-64-1	4.11	0.59	14
5	Methane	74-82-8	< 61	—	—

1 CAS = Chemical Abstract Service.

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

Table 4-2
Tank BY-112 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	0.10	0.08	76
2	n-Dodecane	112-40-3	0.0097	0.0008	8
3	n-Tridecane	629-50-5	0.020	0.006	29

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 BY-112 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	0.0016	0.0003	19
2	Propanenitrile	107-12-0	0.0024	0.0005	19
3	n-Hexane	110-54-3	0.0057	0.0004	7
4	Benzene	71-43-2	0.0020	0.0005	23
5	n-Butanenitrile	109-74-0	0.0049	0.0005	10
6	n-Heptane	142-82-5	0.0062	0.0040	64
7	Toluene	108-88-3	0.015	0.001	9
8	2-Hexanone	591-78-6	0.0054	0.0009	17
9	n-Octane	111-65-9	0.0026	0.0009	35
10	n-Hexanenitrile	628-73-9	0.00093	0.00004	5
11	2-Heptanone	110-43-0	0.0040	0.0003	7
12	n-Nonane	111-84-2	0.0019	0.0004	23
13	n-Heptanenitrile	629-08-3	0.00077	0.00006	7
14	2-Octanone	111-13-7	0.0015	0.0001	4
15	n-Decane	124-18-5	0.0017	0.0001	5
16	n-Undecane	1120-21-4	0.0062	0.0005	8

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 BY-112 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Propanone ⁵ (acetone)	67-64-1	1.00	0.12	12
2	Butanal ⁶	123-72-8	0.016	0.013	87
3	1-Butanol ⁶	71-36-3	0.059	0.001	2
4	2-Pentanone ⁶	107-87-9	0.020	0.004	17
5	n-Pentanenitrile ⁵	110-59-8	0.0012	0.00002	2

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 BY-112 Comparison of Organic Compounds in TST and SUMMA™ Samples--
Analyses by Oak Ridge National Laboratory
and Pacific Northwest 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	< 0.0053	< 0.005	—
Propanone (acetone)	67-64-1	1.0	4.1	122
Ethanenitrile (acetonitrile)	75-05-8	0.10	< 0.005	> 181
Propanenitrile	107-12-0	0.0024	< 0.005	—
n-Butanenitrile	109-74-0	0.0049	< 0.005	—
Benzene	71-43-2	0.0020	< 0.005	—
Toluene	108-88-3	0.015	0.041	93
n-Hexane	110-54-3	0.0057	< 0.005	> 13
n-Heptane	142-82-5	0.0062	< 0.005	> 21
n-Decane	124-18-5	0.0017	< 0.005	—

1 CAS = Chemical Abstract Service.

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

3 Average of 3 samples from PNL.

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

Table 4-6
Tank BY-112 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard ³ Deviation (mg/m ³)
1	Propene ⁴	115-07-1	0.05	0.01
2	Propane	74-98-6	0.063	0.015
3	Cyclopropane	75-19-4	0.12	0.01
4	Ethanal (acetaldehyde)	75-07-0	0.16	0.02
5	Butane	106-97-8	0.12	0.03
6	Ethanol	64-17-5	0.10	0.01
7	n-Pentane	109-66-0	0.073	0.04
8	2-Methyl-2-propanol	75-65-0	0.24	0.02
9	Butanal	123-72-8	0.076	0.006
10	3-Methyl-2-butanone	563-80-4	< 0.04	—
11	1-Butanol	71-36-3	0.087	0.006
12	2-Pentanone	107-87-9	0.077	0.006
13	4,4-Dimethyl-2-pentanone	590-50-1	0.13	0.02
Sum of tentatively identified compounds:			1.31	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples, values listed are estimates.

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

4 Detected in only two samples.

Table 4-7
 Tank BY-112 Tentatively Identified Organic Compounds in TST Samples
 In the Order of Chromatographic Elution --
 Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Methyl nitrite	624-91-9	0.0049	0.0084
2	Cyclopropane	75-19-4	0.011	0.010
3	1-Propene, 2-methyl-	115-11-7	0.046	0.041
4	Methanol	67-56-1	0.36	0.45
5	Ethanol	64-17-5	0.083	0.018
6	Trichlorofluoromethane	75-69-4	0.43	0.06
7	Trichlorofluoromethane	75-69-4	0.076	0.131
8	2-Propanol	67-63-0	0.13	0.12
9	2-Propanol, 2-methyl-	75-65-0	0.0044	0.0076
10	1-Propanol	71-23-8	0.063	0.012
11	Acetic acid	64-19-7	0.072	0.125
12	2-Butanone	78-93-3	0.075	0.066
13	2-Butanone, 3-methyl-	563-80-4	0.016	0.002
14	Nitric acid, propyl ester	627-13-4	0.0047	0.0081
15	2-Pentene, 4-methyl- and others		0.0058	0.0101
16	3-Pentanone	96-22-0	0.0083	0.0072
17	2-Butanone, 3,3-dimethyl-	75-97-8	0.031	0.023
18	2-Butanone, 3,3-dimethyl-	75-97-8	0.013	0.011
19	Formamide	75-12-7	0.0028	0.0049
20	1-Butanol, 3-methyl-	123-51-3	0.0060	0.0052
21	1-Butanol, 3-methyl-, nitrate	543-87-3	0.0028	0.0049
22	2-Pentanone, 4,4-dimethyl-	590-50-1	0.055	0.006
23	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0088	0.0081
24	2,2,4-Trimethyl-3-pentanone	5857-36-3	0.011	0.00008
25	Ethylbenzene	100-41-4	0.0099	0.0004
26	1-Hexanol	111-27-3	0.0052	0.0045
27	Benzene, 1,3-dimethyl-	108-38-3	0.023	0.0007

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	3-Heptanone	106-35-4	0.023	0.002
29	p-Xylene	106-42-3	0.0024	0.0041
30	3-Heptanone, 6-methyl-	624-42-0	0.011	0.0002
31	2-Heptanone, 6-methyl-	928-68-7	0.031	0.002
32	Benzaldehyde	100-52-7	0.015	0.002
33	1-Hexanol, 2-ethyl-	104-76-7	0.0019	0.0034
34	2(3H)-Furanone, dihydro-4,4-dimethyl-	13861-97-7	0.0020	0.0035
35	C10-Alkane		0.020	0.002
36	2-Heptanone, 4,6-dimethyl-	19549-80-5	0.0020	0.0035
37	1-Octanol	111-87-5	0.0022	0.0038
38	Acetophenone	98-86-2	0.0029	0.0051
39	Nonanal	124-19-6	0.0021	0.0037
40	Undecane, 2,6-dimethyl-	17301-23-4	0.0094	0.0023
41	Cyclohexane, hexyl-	4292-75-5	0.0039	0.0067
42	Tridecane, 7-methyl-	26730-14-3	0.026	0.006
43	Methenamine	100-97-0	0.0026	0.0046
44	Undecane, 5-ethyl-	17453-94-0	0.012	0.003
45	Cyclohexane, pentyl-	4292-92-6	0.014	0.004
46	Tridecane, 2-methyl-	1560-96-9	0.0097	0.0019
47	Tridecane, 3-methyl-	6418-41-3	0.0087	0.0017
48	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.073	0.013
49	n-Tetradecane	629-59-4	0.10	0.02
50	Tridecane, 4,8-dimethyl-	55030-62-1	0.011	0.001
51	Cyclohexane, 1,1,3-trimethyl-2-(3-methyl-pentyl)	54965-05-8	0.0097	0.0009
52	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.0018	0.0031
53	n-Hexadecane	544-76-3	0.057	0.006
54	n-Heptadecane	629-78-7	0.045	0.007
55	Cyclohexane, 1,2-dimethyl-3-pentyl-		0.0062	0.0055

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
56	3-Ethyl-2-methyl-2-heptanol		0.0046	0.0040
57	6-Dodecanol	6836-38-0	0.0047	0.0041
58	n-Hexadecane	544-76-3	0.0096	0.0025
59	Butyric acid, thio-, S-decyl ester	2432-55-5	0.013	0.002
60	Diethyl phthalate	84-66-2	0.029	0.012
61	1,1'-Biphenyl, 2,2'-dichloro-	13029-08-8	0.0021	0.004
62	Benzenesulfonamide, N-butyl-	3622-84-2	0.052	0.023
63	Benzenesulfonamide, N-ethyl-4-methyl-	80-39-7	0.0042	0.0073
64	Benzenesulfonamide, N-butyl-	3622-84-2	0.015	0.026
65	Dibutyl phthalate		0.0020	0.0035
66	Isopropyl palmitate	142-91-6	0.012	0.002
Sum of tentatively identified compounds:			2.22	

1 CAS = Chemical Abstract Service.

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

Table 4-8
 Tank BY-112 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)
10	1-Propanol	71-23-8	0.063	0.012
37	1-Octanol	111-87-5	0.0022	0.0038
3	1-Propene, 2-methyl-	115-11-7	0.046	0.041
21	1-Butanol, 3-methyl-, nitrate	543-87-3	0.0028	0.0049
26	1-Hexanol	111-27-3	0.0052	0.0045
20	1-Butanol, 3-methyl-	123-51-3	0.0060	0.0052
33	1-Hexanol, 2-ethyl-	104-76-7	0.0019	0.0034
61	1,1'-Biphenyl, 2,2'-dichloro-	13029-08-8	0.0021	0.004
9	2-Propanol, 2-methyl-	75-65-0	0.0044	0.0076
36	2-Heptanone, 4,6-dimethyl-	19549-80-5	0.0020	0.0035
18	2-Butanone, 3,3-dimethyl-	75-97-8	0.013	0.011
12	2-Butanone	78-93-3	0.075	0.066
13	2-Butanone, 3-methyl-	563-80-4	0.016	0.002
31	2-Heptanone, 6-methyl-	928-68-7	0.031	0.002
15	2-Pentene, 4-methyl- and others		0.0058	0.0101
22	2-Pentanone, 4,4-dimethyl-	590-50-1	0.055	0.006
17	2-Butanone, 3,3-dimethyl-	75-97-8	0.031	0.023
24	2,2,4-Trimethyl-3-pentanone	5857-36-3	0.011	0.00008
34	2(3H)-Furanone, dihydro-4,4-dimethyl-	13861-97-7	0.0020	0.0035
8	2-Propanol	67-63-0	0.13	0.12
56	3-Ethyl-2-methyl-2-heptanol		0.0046	0.0040
16	3-Pentanone	96-22-0	0.0083	0.0072
28	3-Heptanone	106-35-4	0.023	0.002
30	3-Heptanone, 6-methyl-	624-42-0	0.011	0.0002
57	6-Dodecanol	6836-38-0	0.0047	0.0041
11	Acetic acid	64-19-7	0.072	0.125
38	Acetophenone	98-86-2	0.0029	0.0051

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
32	Benzaldehyde	100-52-7	0.015	0.002
27	Benzene, 1,3-dimethyl-	108-38-3	0.023	0.0007
62	Benzenesulfonamide, N-butyl-	3622-84-2	0.052	0.023
63	Benzenesulfonamide, N-ethyl-4-methyl-	80-39-7	0.0042	0.0073
64	Benzenesulfonamide, N-butyl-	3622-84-2	0.015	0.026
59	Butyric acid, thio-, S-decyl ester	2432-55-5	0.013	0.002
35	C10-Alkane		0.020	0.002
41	Cyclohexane, hexyl-	4292-75-5	0.0039	0.0067
45	Cyclohexane, pentyl-	4292-92-6	0.014	0.004
55	Cyclohexane, 1,2-dimethyl-3-pentyl-		0.0062	0.0055
51	Cyclohexane, 1,1,3-trimethyl- 2-(3-methylpentyl)	54965-05-8	0.0097	0.0009
2	Cyclopropane	75-19-4	0.011	0.010
23	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0088	0.0081
65	Dibutyl phthalate		0.0020	0.0035
60	Diethyl phthalate	84-66-2	0.029	0.012
48	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.073	0.013
52	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.0018	0.0031
5	Ethanol	64-17-5	0.083	0.018
25	Ethylbenzene	100-41-4	0.0099	0.0004
19	Formamide	75-12-7	0.0028	0.0049
66	Isopropyl palmitate	142-91-6	0.012	0.002
4	Methanol	67-56-1	0.36	0.45
43	Methenamine	100-97-0	0.0026	0.0046
1	Methyl nitrite	624-91-9	0.0049	0.0084
54	n-Heptadecane	629-78-7	0.045	0.007
53	n-Hexadecane	544-76-3	0.057	0.006
58	n-Hexadecane	544-76-3	0.0096	0.0025
49	n-Tetradecane	629-59-4	0.10	0.02

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
14	Nitric acid, propyl ester	627-13-4	0.0047	0.0081
39	Nonanal	124-19-6	0.0021	0.0037
29	p-Xylene	106-42-3	0.0024	0.0041
6	Trichlorofluoromethane	75-69-4	0.43	0.06
7	Trichlorofluoromethane	75-69-4	0.076	0.131
42	Tridecane, 7-methyl-	26730-14-3	0.026	0.006
46	Tridecane, 2-methyl-	1560-96-9	0.0097	0.0019
47	Tridecane, 3-methyl-	6418-41-3	0.0087	0.0017
50	Tridecane, 4,8-dimethyl-	55030-62-1	0.011	0.001
40	Undecane, 2,6-dimethyl-	17301-23-4	0.0094	0.0023
44	Undecane, 5-ethyl-	17453-94-0	0.012	0.003
Sum of tentatively identified compounds:			2.22	

1 CAS = Chemical Abstract Service.

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

Table 4-9
Tank BY-112 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)
6	Trichlorofluoromethane	75-69-4	0.43	0.06
4	Methanol	67-56-1	0.36	0.45
8	2- Propanol	67-63-0	0.13	0.12
49	n-Tetradecane	629-59-4	0.10	0.02
5	Ethanol	64-17-5	0.083	0.018
7	Trichlorofluoromethane	75-69-4	0.076	0.131
12	2-Butanone	78-93-3	0.075	0.066
48	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.073	0.013
11	Acetic acid	64-19-7	0.072	0.125
10	1-Propanol	71-23-8	0.063	0.012
53	n-Hexadecane	544-76-3	0.057	0.006
22	2-Pentanone, 4,4-dimethyl-	590-50-1	0.055	0.006
62	Benzenesulfonamide, N-butyl-	3622-84-2	0.052	0.023
3	1-Propene, 2-methyl-	115-11-7	0.046	0.041
54	n-Heptadecane	629-78-7	0.045	0.007
31	2-Heptanone, 6-methyl-	928-68-7	0.031	0.002
17	2-Butanone, 3,3-dimethyl-	75-97-8	0.031	0.023
60	Diethyl phthalate	84-66-2	0.029	0.012
42	Tridecane, 7-methyl-	26730-14-3	0.026	0.006
27	Benzene, 1,3-dimethyl-	108-38-3	0.023	0.0007
28	3-Heptanone	106-35-4	0.023	0.002
35	C10-Alkane		0.020	0.002
13	2-Butanone, 3-methyl-	563-80-4	0.016	0.002
32	Benzaldehyde	100-52-7	0.015	0.002
64	Benzenesulfonamide, N-butyl-	3622-84-2	0.015	0.026
45	Cyclohexane, pentyl-	4292-92-6	0.014	0.004
59	Butyric acid, thio-, S-decyl ester	2432-55-5	0.013	0.002

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
18	2-Butanone, 3,3-dimethyl-	75-97-8	0.013	0.011
66	Isopropyl palmitate	142-91-6	0.012	0.002
44	Undecane, 5-ethyl-	17453-94-0	0.012	0.003
24	2,2,4-Trimethyl-3-pentanone	5857-36-3	0.011	0.00008
50	Tridecane, 4,8-dimethyl-	55030-62-1	0.011	0.001
2	Cyclopropane	75-19-4	0.011	0.010
30	3-Heptanone, 6-methyl-	624-42-0	0.011	0.0002
25	Ethylbenzene	100-41-4	0.0099	0.0004
46	Tridecane, 2-methyl-	1560-96-9	0.0097	0.0019
51	Cyclohexane, 1,1,3-trimethyl- 2-(3-methylpentyl)	54965-05-8	0.0097	0.0009
58	n-Hexadecane	544-76-3	0.0096	0.0025
40	Undecane, 2,6-dimethyl-	17301-23-4	0.0094	0.0023
23	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0088	0.0081
47	Tridecane, 3-methyl-	6418-41-3	0.0087	0.0017
16	3-Pentanone	96-22-0	0.0083	0.0072
55	Cyclohexane, 1,2-dimethyl-3-pentyl-		0.0062	0.0055
20	1-Butanol, 3-methyl-	123-51-3	0.0060	0.0052
15	2-Pentene, 4-methyl- and others		0.0058	0.0101
26	1-Hexanol	111-27-3	0.0052	0.0045
1	Methyl nitrite	624-91-9	0.0049	0.0084
57	6-Dodecanol		0.0047	0.0041
14	Nitric acid, propyl ester	627-13-4	0.0047	0.0081
56	3-Ethyl-2-methyl-2-heptanol		0.0046	0.0040
9	2-Propanol, 2-methyl-	75-65-0	0.0044	0.0076
63	Benzenesulfonamide, N-ethyl-4-methyl-	80-39-7	0.0042	0.0073
41	Cyclohexane, hexyl-	4292-75-5	0.0039	0.0067
38	Acetophenone	98-86-2	0.0029	0.0051
21	1-Butanol, 3-methyl-, nitrate	543-87-3	0.0028	0.0049

WHC-SD-WM-ER-441 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
19	Formamide	75-12-7	0.0028	0.0049
43	Methenamine	100-97-0	0.0026	0.0046
29	p-Xylene	106-42-3	0.0024	0.0041
37	1-Octanol	111-87-5	0.0022	0.0038
39	Nonanal	124-19-6	0.0021	0.0037
61	1,1'-Biphenyl, 2,2'-dichloro	13029-08-8	0.0021	0.004
36	2-Heptanone, 4,6-dimethyl-	19549-80-5	0.0020	0.0035
34	2(3H)-Furanone, dihydro-4,4-dimethyl-	13861-97-7	0.0020	0.0035
65	Dibutyl phthalate		0.0020	0.0035
33	1-Hexanol, 2-ethyl-	104-76-7	0.0019	0.0034
52	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.0018	0.0031
Sum of tentatively identified compounds:			2.22	

1 CAS = Chemical Abstract Service.

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