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TANK 241BY104 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
4/1994 & 6/1994

COMPLETE

ENGINEERING CHANGE NOTICE

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ENGINEERING CHANGE NOTICE				Page 2 of 2	1. ECN (use no. from pg. 1) 625438
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Functional Design Criteria	☐	Stress/Design Report	☐	Health Physics Procedure	☐
Operating Specification	☐	Interface Control Drawing	☐	Spares Multiple Unit Listing	☐
Criticality Specification	☐	Calibration Procedure	☐	Test Procedures/Specification	☐
Conceptual Design Report	☐	Installation Procedure	☐	Component Index	☐
Equipment Spec.	☐	Maintenance Procedure	☐	ASME Coded Item	☐
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OM Manual	☐	Operational Safety Requirement	☐	ICRS Procedure	☐
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WHC Information Release Administration Specialist:

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7. Abstract

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

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Tank 241-BY-104 Headspace Gas and Vapor Characterization Results for Samples Collected in April 1994 and June 1994

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Contents

1.0 INTRODUCTION	1
1.1 Characterization Objectives	1
1.2 Characterization Data Criteria	1
1.3 Sampling Overview	2
1.4 Tank Headspace Dynamics	2
2.0 SAMPLING EVENT	3
2.1 April 1994 <i>In Situ</i> Sampling Event	3
2.2 June 1994 Vapor Sampling System Sampling Event	3
3.0 INORGANIC GASES AND VAPORS	4
3.1 Ammonia, Hydrogen, and Nitrous Oxide	4
3.2 Carbon Dioxide and Carbon Monoxide	4
3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium	5
3.4 Hydrogen Cyanide	5
3.5 Discussion of Inorganic Gases and Vapors	5
4.0 ORGANIC VAPORS	7
4.1 Positively Identified Organic Analytes	7
4.2 Tentatively Identified Organic Analytes	8
4.3 Total Nonmethane Organic Carbon	9
4.4 Discussion of Organic Analytes	9
5.0 SUMMARY	11
6.0 REFERENCES	12

Acronyms and Abbreviations

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

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Tank 241-BY-104 Headspace Gas and Vapor Characterization Results
for Samples Collected in April 1994 and June 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BY-104 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). This report primarily discusses results from the June 1994 sampling event, but also includes selected results of the April 1994 sampling event. The tank BY-104 headspace was sampled in April 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in June 1994 in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

1.2 Characterization Data Criteria

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

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank BY-104, specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995a).

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

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

1.3 Sampling Overview

Tank BY-104 was vapor sampled in April 1994 using the *in situ* sampling (ISS) method, and again in June 1994 using the more robust vapor sampling system (VSS) method. Because the ISS sample volume flow measurement used during the April 1994 event was inherently less accurate than that of the VSS, the sorbent trap samples from the ISS event are not considered to be equivalent to those from the VSS sampling event (Huckaby et al. 1995). Furthermore, there are other discrepancies between results from the ISS and VSS methods that are not understood (Huckaby 1994a), and until the ISS method has been validated and the discrepancies resolved, results from early ISS events should be considered suspect.

Nevertheless, a brief description of the ISS event and hydrogen cyanide sampling results from the April 1994 ISS event are presented below, because this analyte was not sampled for during the VSS event. Huckaby et al. (1995) describe the bases for using the ISS method for hydrogen cyanide, and why it was not sampled for during the VSS event. All other results presented here are from the June 1994 VSS sampling event.

Samples collected are thought to have been representative of the tank headspace when the tank was sampled (Meacham et al. 1995), and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment has been made of how the tank BY-104 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in passively ventilated tanks, such as tank BY-104 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank BY-104 is the first tank in a 3-tank cascade with tanks BY-105 and BY-106. It is connected to tank BY-105 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. Tanks BY-105 and BY-106 are connected by a similar line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank BY-105 or BY-106 may be transferred to tank BY-104 (unless the cascade lines are obstructed).

The cascade of tanks BY-104, BY-105, and BY-106 is passively ventilated, which means that the tanks are allowed to exhale air, waste gases, and vapors as the barometric pressure falls, and inhale ambient air as the barometric pressure rises. Each of these tanks has its own filtered breather riser. Barometric pressure typically rises and falls on a diurnal cycle, producing an average daily exchange of air equal to about 0.46 % of each tank headspace (Huckaby 1994b). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

2.1 April 1994 *In Situ* Sampling Event

Tank BY-104 was sampled using ISS methods on April 22, 1994 by WHC Sampling and Mobile Laboratories. This sampling was conducted to satisfy requirements of *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991). Samples for hydrogen cyanide were collected from a point approximately 7.3 m below the top of the flange on riser 4, between 12:00 noon and 1:00 p.m.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1994) provides field sampling information for the tank BY-104 April 1994 ISS event, and Mahon (1995) provides revised sample volume measurements. In addition to the hydrogen cyanide results presented below, Pool et al. (1995) provide sample preparation and analysis results for selected organic and inorganic vapors, and Rasmussen (1994a) provides SUMMA™ canister analysis results from the April 1994 ISS event.

2.2 June 1994 Vapor Sampling System Sampling Event

Headspace vapor samples were collected from tank BY-104 using the VSS on June 24, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by the sample and analysis plan¹ (WHC 1995b, Appendix A). Tank BY-104 was the first tank to be vapor sampled after the effectiveness of the VSS had been demonstrated on tank C-103. Air from the tank BY-104 headspace was withdrawn via a heated sampling probe mounted in riser 10A, and transferred via heated tubing to the VSS sampling manifold.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories. The 46 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 10 trip 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).

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

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,2} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Sorbent traps were prepared and analyzed by PNL, SUMMATM canisters were analyzed by OGIST. Reports by Clauss et al. (1994) and Rasmussen (1994b) describe sample preparation and analyses.

Analyses of the VSS event inorganic vapor sorbent traps were performed within 25 days of sample collection, and analyses of the ISS event hydrogen cyanide sorbent traps were completed within 52 days after sample collection (Ligotke 1995, Pool et al. 1995). These analyses were performed within the allowed 60-day holding time specified in the WHC quality assurance project plan (Keller 1994). All PNL results were produced at PNL quality assurance impact level 3.

OGIST did not have a WHC-approved quality assurance project plan at the time of analyses, and OGIST results should be considered secondary results. OGIST data have been placed in brackets in Table 3-1 and elsewhere in this report to indicate them as secondary data. OGIST started analyses 33 days after collection of samples.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration in tank BY-104, 248 ppmv, is a typical value for the passively ventilated tanks. Ammonia concentrations have been measured to be as high as about 1040 ppmv in tank BY-108 (McVeety et al. 1995). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 248 ppmv corresponds to less than 0.2 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

Hydrogen was measured to be an average [295 ppmv] in 3 SUMMATM canister samples by OGIST. In general, hydrogen is of concern as a fuel. The measured 295 ppmv of hydrogen in tank BY-104, however, represents only about 0.7 % of the LFL for hydrogen in air, and is not a flammability concern at this level.

Nitrous oxide was present in SUMMATM canister samples at an average of [201 ppmv]. This is a typical value for a passively ventilated tank, such as tank BY-104. 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-104 headspace.

3.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, [10.5 ppmv], is markedly lower than normal ambient air concentrations of about 350 to 400 ppmv. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. Though lower than in most other passively ventilated tanks that

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

have been sampled, the carbon dioxide concentration in tank BY-104 is within the normal range of these tanks.

Carbon monoxide in the tank BY-104 headspace, at about [1.0 ppmv], is more concentrated than it is in ambient air, where it typically is about 0.05 to 0.15 ppmv. Carbon monoxide may be a decomposition of organic waste in tank BY-104.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BY-104 headspace were determined to be 0.29 ppmv and ≤ 0.07 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH interstitial liquid in tank BY-104. 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-104 headspace.

The water vapor concentration of tank BY-104 was determined to be about 14.1 mg/L, at the measured tank headspace temperature of 26 °C and pressure of 994 mbar (747 torr), (WHC 1995b). This corresponds to water vapor partial pressure of 19.4 mbar (14.6 torr), to a dew point of 17.0 °C, and to a relative humidity of 58 %.

Tritium was tested for using silica gel sorbent traps. 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. Analysis of the silica gel, which would have trapped approximately 32 mg of water vapor, indicated the total activity of the sample to be below the method detection limit of 50 pCi (WHC 1995b).

3.4 Hydrogen Cyanide

Analysis of the hydrogen cyanide specific sorbent traps indicated the concentration of this analyte to ≤ 0.007 ppmv in all 3 samples. The absence of hydrogen cyanide at measurable concentrations is consistent with the expectation that an acid gas, such as hydrogen cyanide, would not exist at significant concentrations above the caustic waste in tank BY-104. No hydrogen cyanide has been detected in any of the 10 waste tank headspaces sampled for this analyte.

3.5 Discussion of Inorganic Gases and Vapors

Aside from water vapor and carbon dioxide, the most abundant waste constituents in the tank BY-104 headspace are ammonia, hydrogen, and nitrous oxide. These have been detected in most tank headspaces sampled to date, and usually are 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 2 % for ammonia to 14 % for nitric oxide. 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-105 and BY-106 could be transferred to tank BY-104 via the cascade lines. If significant exchange of selected inorganic gases and vapors were taking place between adjacent tanks, either their headspace compositions would be very similar (if the exchange was mutual), or all constituents detected in one tank would be at or equal or higher concentrations in the other tank (if air flowed predominantly from 1 tank to the other). Consideration of data in Table 3-2 indicates that the ammonia, hydrogen, and nitrous oxide detected in tank BY-104 must coming from the waste in that tank. The data do not otherwise support or rule out the potential transfer of air, gases, and vapors.

4.0 ORGANIC VAPORS

Organic vapors in the tank BY-104 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. None of the positively or tentatively identified organic analytes were at or above levels of concern. 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. (1994) and Clauss et al. (1994). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIST (EPA 1988, Rasmussen 1994b).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-104. These results were produced at PNL quality assurance impact level 3, and all PNL organic analyses were completed 34 days after sample collection (Ligotke 1995), well within the allowed 60-day holding time (Keller 1994). No holding time study has been performed to determine the stability of organic analytes in SUMMA™ canisters in the chemical matrix of the tank samples.

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

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

4.1 Positively Identified Organic Analytes

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

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list included 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of vapor data on tank C-103.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL. PNL performed analyses according to the EPA TO-14 methodology. Only 4 of the 40 TO-14 analytes were observed to be above the general 0.002 ppmv quantitation limit of the analyses (Clauss et

al. 1994 provide the complete TO-14 analyte list). Averages reported are from analyses of 3 SUMMA™ canister samples except where noted.

ORNL positively identified and quantitated 26 of 27 analytes selected by WHC, (1,1-dichloroethene was below its detection limit). Despite calibration of the instrument over about a 20-fold concentration range, 19 of the 26 positively identified compounds were outside of the calibration range in at least 1 of the TST samples. The 7 quantitated analytes, and their average reported concentration from 4 TSTs, are given in Table 4-2. Tables 4-3 and 4-4 list the positively identified compounds which were not quantitated because their measured value in at least 1 TST was outside the calibration range. One of these compounds, butanal, is listed separately in Table 4-4 because analyses were performed after the ORNL practical holding time had elapsed. Results in Tables 4-3 and 4-4 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. The reported practical holding time of butanal is 1 day (Jenkins et al. 1995b), and analyses of TSTs were not completed until 9 days after sample collection (Jenkins 1995b). It should be noted that the practical holding time study was done much later than the tank BY-104 analyses, and at the time of analysis the contractual holding time for the TST samples was 60 days.

Table 4-5 lists the 3 analytes common to both the ORNL and PNL analyses (dichloromethane, benzene, and toluene) with their average measured concentrations. The ORNL and PNL results agree for dichloromethane, but differ by more than a factor of 4 for toluene, and by more than a factor of 12 for benzene (Table 4-5). Though these differences are greater than the allowed $\pm 30\%$ analytical accuracy, they are not unreasonable given that fundamentally different sampling devices and analytical methods were used.

The 3 most abundant organic compounds in the tank BY-104 headspace are methane, propanone, and 1-butanol. At 8.2 ppmv, the methane concentration is about 4 times higher than its normal ambient air concentration. Methane is probably formed during the chemical and radiolytic degradation of organic wastes in tank BY-104. Methane is not a constituent of toxicological concern, and its LFL in air is about 5 vol%. This places the 8.2 ppmv of methane in tank BY-104 at less than 0.02 % of its LFL. Propanone, at 1.2 ppmv, and 1-butanol, at 1.0 ppmv, are the only other organic constituents at or above the 1 ppmv level.

4.2 Tentatively Identified Organic Analytes

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

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and SUMMA™ samples. Analyses of the samples are designed to recover,

separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (e.g., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (e.g., butanal) from SUMMA™ samples has been problematic.

The organic compounds tentatively identified in SUMMA™ canister samples by PNL are listed, with their estimated concentrations, in Table 4-6. Compounds are listed in Table 4-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table 4-7. Compounds are listed in Table 4-7 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 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 locating any given compound may be difficult, 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 PNL and ORNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1994), respectively, and should be reviewed before this data are used for decision making. Results in Tables 4-6 through 4-9 are presented in terms of observed peaks, and are not adjusted for the occurrence of chromatographically split peaks (e.g., Cmpd # 3 and 4 in Table 4-7) or the assignment of the same chemical identity to more than 1 peak (e.g., 24 and 28 in Table 4-7). In these instances, the estimated concentration of a compound identified in different peaks is simply the sum of the individual peak estimates.

Concentrations given in Tables 4-6 through 4-8 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

4.3 Total Nonmethane Organic Carbon

OGIST measured the TNMOC concentration in 3 SUMMA™ canister samples using the EPA TO-12 method (Rasmussen 1994b). The sample mean was [60.8 mg/m³], with a standard deviation of [5.9 mg/m³]. Compared to other passively ventilated tanks that have been sampled, tank BY-104 has relatively high concentrations of volatile and semivolatile organic waste.

4.4 Discussion of Organic Analytes

Some of the compounds listed in Tables 4-1 through 4-9 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are tributyl phosphate, which was used as an extractant in several Hanford processes; dibutyl butylphosphonate, which was a contaminant of tributyl phosphate; and the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-undecane, n-dodecane, n-tridecane, and

n-pentadecane) and branched and cyclic alkanes (e.g., methylated decahydronaphthalenes, cyclopentanes, and cyclohexanes) with similar boiling points that were used as a diluent for tributyl phosphate.

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

Examination of the compounds listed in Tables 4-1 through 4-9 suggests many of the volatile species (presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom. For example, most alkenes listed have their double bond between the first and second carbon atoms, and ketones generally have the double bonded oxygen atom on the second carbon atom.

As observed in other NPH-containing waste tanks, there are many small cyclic compounds, specifically cyclopropanes, cyclopentanes, and furans. The presence of these suggest that organic radicals, formed in the radiation field of the tank, play a role in the degradation of the semivolatile compounds.

5.0 SUMMARY

The tank BY-104 headspace was sampled in April 1994 and June 1994 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the April 1994 event and essentially all results from the June 1994 event have been reported. It was determined that no headspace constituents exceeded the flammability notification limits, but that ammonia, measured to be 248 ppmv, exceeded the 150 ppmv industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank BY-104 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	2.0	Organic vapors	4 tank air samples + 2 trip blanks
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous oxide, Carbon dioxide, Carbon monoxide, Organic vapors	3 tank air samples
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	5 tank air samples + 2 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen dioxide	10 tank air samples + 2 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric oxide	10 tank air samples + 2 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	10 tank air samples + 2 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	2.0	Tritium-substituted water vapor	1 tank air sample

Table 3-1
Tank BY-104 Inorganic Gas and Vapor Concentrations --
Analyses by Oregon Graduate Institute of Science and Technology and Pacific Northwest Laboratory

Compound	CAS ¹ Number	Sample Type	Number of samples	Average ² (ppmv)	Standard Deviation ² (ppmv)	RSD ^{2,3} (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	5	248	5	2
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	[10.5]	[0.7]	[7]
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	[1.0]	[0.11]	[11]
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	[295]	[15]	[5]
Hydrogen Cyanide ⁴ , HCN	74-90-8	Sorbent Trap	3	≤ 0.007	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	10	0.29	0.04	14
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	10	≤ 0.07	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	[201]	[8]	[4]
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	10	19,500 (14.1 mg/L)	1,100 (0.8 mg/L)	6

1 CAS = Chemical Abstract Service.

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

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

4 Results for hydrogen cyanide are from the April 1994 ISS event.

Table 3-2
Comparison of Tank BY-104, BY-105, and BY-106 Headspace Constituents --
Inorganic Analyses by Oregon Graduate Institute of Science and Technology,
and Organic Analyses by Oak Ridge National Laboratory¹

Tank:	BY-104	BY-105 ²	BY-106 ³
Date sampled, (mo/day/yr)	6/24/94	7/7/94	7/8/94
Headspace temperature, (°C)	26	26	27
Ammonia, (ppmv)	248	43	74
Hydrogen, (ppmv)	[295]	[47.9]	[45.5]
Carbon dioxide, (ppmv)	[10.5]	[94]	[47.6]
Carbon monoxide, (ppmv)	[1.0]	[0.38]	[0.45]
Nitric oxide, (ppmv)	0.29	0.10	0.13
Nitrogen dioxide, (ppmv)	≤ 0.07	≤ 0.02	0.05
Nitrous oxide, (ppmv)	[201]	[49.5]	[70.6]
Water vapor, (mg/m ³)	14.1	14.9	14.7
Water vapor, (% relative humidity)	58	76	57
Ethanenitrile (acetonitrile), (ppmv)	(0.33)	(0.081)	(0.12)
Propanone (acetone), (ppmv)	(1.2)	(0.25)	(0.37)
1-Butanol, (ppmv)	(1.0)	(0.70)	(0.34)
n-Dodecane, (ppmv)	(0.058)	(0.0081)	(0.0065)
n-Tridecane, (ppmv)	(0.084)	(0.010)	(0.0069)
Total nonmethane organic carbon, (mg/m ³)	[60.8]	[12.7]	[9.9]

1 Where PNL inorganic gas or vapor data was unavailable, OGIST results are given. OGIST results are in brackets to indicate the data should be considered secondary results. 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.

Table 4-1
Tank BY-104 Quantitatively Measured Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Methane ⁴	74-82-8	[8.2]	[0.3]	[4]
2	Dichlorodifluoromethane	75-71-8	0.0008	0.0002	19
3	Chloromethane (Methyl chloride)	74-87-3	0.0017 ⁵	--	--
4	Trichlorofluoromethane	75-69-4	0.360	0.046	13
5	Dichloromethane (Methylene chloride)	75-09-2	0.0018 ⁵	--	--
6	Benzene	71-43-2	0.0031	0.0007	22
7	Toluene	108-88-3	0.010	0.003	24
8	Tetrachloroethene	127-18-4	0.0016 ⁵	--	--
9	Ethylbenzene	100-41-4	0.0018	0.0001	5
10	1,3-Dimethylbenzene (m-xylene) + 1,4-Dimethylbenzene (p-xylene) ⁶	108-38-3 106-42-3	0.0048	0.0002	4
11	1,2-Dimethylbenzene (o-xylene)	95-47-6	0.0017	0.0001	8
Sum of organic compounds:					

1 CAS = Chemical Abstract Service.

2 Average of 3 samples.

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

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

5 Result from only 1 sample, < 0.002 ppmv in other samples.

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

Table 4-2
Tank BY-104 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	Propanenitrile	107-12-0	0.016	0.003	21
2	Benzene	71-43-2	0.042	0.011	27
3	Butanenitrile	109-74-0	0.020	0.002	11
4	Pentanenitrile	110-59-8	0.012	0.002	19
5	Hexanenitrile	628-73-9	0.010	0.001	12
6	Heptanenitrile	629-08-3	0.007	0.0007	11
7	2-Octanone	111-13-7	0.015	0.002	11

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

2 CAS = Chemical Abstract Service.

3 Average of 4, 2-L TST samples.

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

Table 4-3
Tank BY-104 Positively Identified Organic Compound 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	0.002	0.0004	20
2	Ethanenitrile (Acetonitrile)	75-05-8	0.33	0.086	26
3	Propanone (Acetone)	67-64-1	1.2	0.293	24
4	n-Hexane	110-54-3	0.32	0.027	9
5	1-Butanol	71-36-3	1.0	0.090	9
6	2-Pentanone	107-87-9	0.16	0.016	10
7	n-Heptane	142-82-5	0.12	0.011	9
8	Toluene	108-88-3	0.041	0.012	30
9	2-Hexanone	591-78-6	0.065	0.010	16
10	n-Octane	111-65-9	0.059	0.006	11
11	2-Heptanone	110-43-0	0.048	0.005	11
12	n-Nonane	111-84-2	0.028	0.001	5
13	Octanenitrile	124-12-9	0.003	0.0002	8
14	Nonanenitrile	2243-27-8	0.002	0.0004	16
15	n-Dodecane	112-40-3	0.058	0.003	6
16	n-Tridecane	629-50-5	0.084	0.008	10
17	Tributyl phosphate (TBP)	126-73-8	0.00082	0.00009	
18	Dibutyl butylphosphonate (DBBP)	75-46-4	0.000087	0.00001	

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

2 CAS = Chemical Abstract Service.

3 Average of 4, 2-L TST samples.

4 RSD = relative standard deviation.

Table 4-4
Tank BY-104 Positively Identified Organic Compound 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	0.16	0.038	24

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

2 CAS = Chemical Abstract Service.

3 Average of 4, 2-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.

Table 4-5
Tank BY-104 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory
and Oak Ridge National Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	PRD ⁴ (%)
Dichloromethane (Methylene chloride)	75-09-2	0.002	0.0018	10
Benzene	71-43-2	0.042	0.0031	172
Toluene	108-88-3	0.041	0.010	122

1 CAS = Chemical Abstract Service.

2 Average of 4, 2-L TST samples analyses.

3 Average of 3 samples analyses.

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

Table 4-6
Tank BY-104 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses Conducted by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propene	115-07-1	1.35	0.66
2	Propane	74-98-6	0.60	0.28
3	Cyclopropane	75-19-4	0.17	0.08
4	2-Methylpropane	75-28-5	0.35	0.17
5	2-Butene	107-01-7	0.65	0.33
6	n-Butane	106-97-8	0.76	0.37
7	2-Methylpropene	115-11-7	0.15	0.08
8	2-Methyl-2-Butene ³	513-35-9	0.05	0.09
9	Propanone (acetone)	67-64-1	1.99	1.01
10	1-Pentene	109-67-1	0.30	0.19
11	n-Pentane	109-66-0	0.79	0.57
12	4-Methyl-1-pentene ³	691-37-2	0.05	0.09
13	2-Methylpentane	107-83-5	1.03	0.22
14	Butanal	123-72-8	0.16	0.03
15	Butanone	78-93-3	0.51	0.11
16	3-Methylpentane	96-14-0	0.23	0.02
17	1-Hexene	107-01-7	0.23	0.03
18	n-Hexane	110-54-3	0.79	0.19
19	Tetrahydrofuran	109-99-9	0.20	0.04
20	Methylcyclopentane	96-37-7	0.11	0.01
21	1-Butanol	71-36-3	0.68	0.15
22	2-Pentanone	107-87-9	0.45	0.19
23	3-Methylhexane	589-34-4	0.35	0.06
24	Heptene		0.11	0.03
25	n-Heptane	142-82-5	0.53	0.10
26	C ₆ Ketone ³		0.03	0.05
27	Methylcyclohexane	108-87-2	0.10	0.01
28	2-Methylheptane	592-27-8	0.20	0.03
29	2-Hexanone	591-78-6	0.18	0.03
30	n-Octane	111-65-9	0.22	0.03

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
31	C ₉ Alkane		0.09	0.01
32	1-Heptanol ⁴	111-70-6	0.10	0.02
33	Trimethylcyclohexane ⁴		--	--
34	3-Heptanone	106-35-4	0.17	0.02
35	2-Heptanone	110-43-0	0.16	0.03
36	2-Butoxyethanol	111-76-2	0.10	0.02
37	n-Nonane	111-84-2	0.14	0.02
38	6-Methylheptanone		0.31	0.05
39	2-Octanone	111-13-7	0.05	0.05
40	n-Decane	124-18-5	0.14	0.03
41	C ₁₁ Alkane		0.03 ²	0.05
42	n-Undecane	1120-21-4	0.37	0.08
43	Methyldodecahydronaphthalene		0.09	0.02
44	C ₅ Cyclohexane		0.13	0.02
45	C ₁₀ Alkane		0.14	0.03
46	Methyldodecahydronaphthalene		0.17	0.02
47	C ₁₂ Alkane		0.12	0.02
48	n-Dodecane	112-70-3	1.58	0.37
49	C ₁₂ Alkane		0.14	0.27
50	Alkane		0.64	0.12
51	C ₁₃ Alkane		0.15	0.30
52	n-Tridecane	629-50-5	0.22	0.52
53	C ₁₄ Alkane		0.12	0.20
54	n-Tetradecane	629-59-4	0.13	0.22
55	C ₁₅ Alkane		0.04	0.05
56	n-Pentadecane	629-62-9	0.02	0.02
Sum of tentatively identified compounds:			26.74	

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero, values listed are estimates.

3. Detected in only 1 sample, average includes zeros of other samples.

4. Compound #32 and #33 were coelutents, concentration given for #32 is that of their sum.

Table 4-7
Tank BY-104 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-Butene	106-98-9	0.66	0.77
2	Butane	106-97-8	0.73	0.85
3	1-Propene, 2-methyl-	115-11-7	0.12	0.08
4	1-Propene, 2-methyl-	115-11-7	0.26	0.18
5	2-Butene	107-01-7	0.089	0.060
6	1-Butene, 3-methyl-	563-45-1	0.083	0.096
7	Butane, 2-methyl-	78-78-4	0.90	0.60
8	2-Propanol and others		0.14	0.27
9	Methane, trichlorofluoro-	75-69-4	0.58	0.39
10	Cyclopropane, ethyl-	1191-96-4	0.76	0.33
11	C5-Alkane		1.0	2.0
12	Mixture of pentene and pentyne		0.29	0.18
13	2-Propanol	67-63-0	0.14	0.27
14	2-Pentene, (Z)	627-20-3	0.095	0.015
15	Cyclopentane	287-92-3	0.16	0.11
16	Cyclopropane, 1,1-dimethyl-	1630-94-0	0.091	0.063
17	1,3-Butadiene, 2-methyl-	78-79-5	0.12	0.03
18	Mixture of 2-propanenitrile & C6-Alkane		0.10	0.02
19	1,3-Butadiene, 2-methyl-	78-79-5	0.035	0.041
20	1-Pentene, 4-methyl-	691-37-2	0.36	0.07
21	Cyclobutanone	1191-95-3	0.15	0.04
22	Pentane, 2-methyl-	107-83-5	2.0	0.3
23	C6-Alkene		0.36	0.18
24	1-Hexene	592-41-6	0.015	0.030
25	C6-Alkene		0.012	0.024
26	Pentane, 3-methyl-	96-14-0	0.48	0.11
27	1-Pentene, 2-methyl-	763-29-1	0.22	0.02
28	1-Hexene	592-41-6	0.49	0.10
29	3-Buten-2-one	78-94-4	0.16	0.02

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
30	2-Butanone	78-93-3	1.4	0.6
31	Furan, 2-methyl-	534-22-5	0.019	0.039
32	2-Hexene, (E)	4050-45-7	0.090	0.004
33	2-Butene, 2,3-dimethyl-	563-79-1	0.12	0.03
34	2-Butanol and others		0.030	0.061
35	2-Propanol	67-63-0	0.063	0.073
36	Cyclopropane, propyl-	2415-72-7	0.11	0.02
37	Mixture		0.11	0.01
38	Cyclopropane, (1-methylethyl)-	3638-35-5	0.29	0.06
39	2-Propanol	67-63-0	0.46	0.07
40	Propanenitrile, 2-methyl-	78-82-0	0.015	0.031
41	Tetrahydrofuran	109-99-9	0.79	0.11
42	1,3-Pentadiene, 2-methyl-	1118-58-7	0.25	0.05
43	1,4-Hexadiene	592-45-0	0.14	0.03
44	2-Butanol, 2-methyl-	75-85-4	0.035	0.044
45	1,4-Hexadiene and siloxane	592-45-0	0.017	0.034
46	C7-Alkene		0.041	0.048
47	1,5-Hexadiene	592-42-7	0.12	0.04
48	Cyclohexane	110-82-7	0.054	0.037
49	Pentanal	110-62-3	0.021	0.042
50	2-Butanone, 3-methyl-	563-80-4	0.052	0.012
51	Hexane, 2-methyl-	591-76-4	0.17	0.01
52	C8-Alkene		0.017	0.012
53	Formic acid, butyl ester	592-84-7	0.0075	0.0151
54	1,4-Hexadiene	592-45-0	0.012	0.015
55	3-Buten-2-one, 3-methyl-	814-78-8	0.019	0.038
56	2-Propenal, 2-methyl-	78-85-3	0.049	0.010
57	Cyclopentane, 1,2-dimethyl-	2452-99-5	0.050	0.005
58	3-Heptene, (E)	14686-14-7	0.018	0.014
59	Alkanol		0.030	0.005
60	2-Heptene	592-77-8	0.046	0.015
61	2,3-Pentanedione	600-14-6	0.018	0.036

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
62	Furan, 2,5-dimethyl-	625-86-5	0.0097	0.0193
63	3-Pentanone, 2-methyl-	565-69-5	0.052	0.037
64	2-Heptene (E)	592-77-8	0.034	0.007
65	Cyclohexane, methyl-	108-87-2	0.17	0.02
66	Nitric Acid, ethyl ester	625-58-1	0.0046	0.0092
67	Unknown		0.017	0.020
8	Alkene and others		0.033	0.024
69	Alkane and others		0.0070	0.0141
70	Cyclopentane, ethyl-	1640-89-7	0.011	0.022
71	2-Pentanol, 2-methyl-	590-36-3	0.050	0.005
72	Cyclopentane, 1,2,4-trimethyl-, (1.alpha.,2.alpha.,4.beta.)-	4850-28-6	0.022	0.015
73	Pentanal, 2-methyl-	123-15-9	0.23	0.03
74	Siloxane and others		0.045	0.030
75	3-Pentanone, 2-methyl-	565-69-5	0.0081	0.0162
76	2-Pentanone, 3-methyl-	565-61-7	0.032	0.026
77	Unknown		0.014	0.028
78	Butane, 2,2,3,3-tetramethyl-	594-82-1	0.017	0.034
79	1-Pentene, 3,4-dimethyl-	7385-78-6	0.063	0.012
80	Alkane and siloxane		0.059	0.119
81	Heptane, 2-methyl-	592-27-8	0.15	0.30
82	4-Pentenal, 2-ethyl-		0.018	0.035
83	C8-Alkane		0.077	0.153
84	Heptane, 4-methyl-	589-53-7	0.12	0.02
85	Alkene		0.32	0.04
86	Alkanol		0.023	0.034
87	1,4-Hexadiene, 4-methyl-	1116-90-1	0.0086	0.0172
88	2-Hexanone, 5-methyl-	110-12-3	0.045	0.007
89	3-Hexanone	589-38-8	0.14	0.02
90	C7-Alkene		0.0099	0.0199
91	2-Ethyl-5-methylfuran	1703-52-2	0.012	0.025
92	Alkanol		0.0065	0.0130

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
93	2-Hexanal	66-25-1	0.0066	0.0133
94	3-Octene, (E)	14919-01-8	0.13	0.19
95	Tetrachloroethylene	127-18-4	0.012	0.014
96	Acetic acid, butyl ester	123-86-4	0.023	0.005
97	Hexamethylcyclotrisiloxane	541-05-9	0.014	0.016
98	Pyridine, 4-methyl-	108-89-4	0.0046	0.0091
99	2-Hexenal	505-57-7	0.0064	0.0127
100	Mixture		0.0062	0.0123
101	Heptane, 2,6-dimethyl-	1072-05-5	0.13	0.02
102	Phenol, 2-methyl-	95-48-7	0.010	0.020
103	3-Penten-1-ol and others		0.019	0.013
104	Cyclohexane, ethyl-	1678-91-7	0.042	0.004
105	C7-Alkanone		0.0052	0.0104
106	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.061	0.018
107	Mixture		0.086	0.020
108	Mixture		0.076	0.008
109	2-Hexanone, 4-methyl-	105-42-0	0.14	0.10
110	C7-Alkanone		0.050	0.100
111	Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)-	1795-27-3	0.0056	0.0112
112	Heptane, 2,3-dimethyl-	3074-71-3	0.036	0.008
113	Heptane, 2,6-dimethyl-	1072-05-5	0.045	0.031
114	C9-Alkane		0.17	0.06
115	Benzene, 1,2-dimethyl-	95-47-6	0.039	0.079
116	4-Octen-3-one	14129-48-7	0.0045	0.0089
117	Butane, 1,1'-oxybis-	142-96-1	0.037	0.028
118	3-Heptanone	106-35-4	0.14	0.08
119	Styrene	100-42-5	0.026	0.009
120	Benzene, 1,2-dimethyl-	95-47-6	0.029	0.030
121	Pentane, 1-methoxy-	628-80-8	0.037	0.006
122	Cyclohexane, 1-ethyl-4-methyl, cis	4926-78-7	0.0019	0.0039
123	Tetramethylcyclohexane		0.0051	0.0060

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
124	Cyclohexane, 1-ethyl-4-methyl-trans-	6236-88-0	0.0025	0.0051
125	C8-Alkanone		0.049	0.003
126	Mixture		0.010	0.001
127	Mixture		0.047	0.008
128	Alkanol		0.0078	0.0091
129	Octane, 2,6-dimethyl-	2051-30-1	0.11	0.03
130	2-Heptanone,4-methyl-	6137-06-0	0.026	0.030
131	Heptane, 3-ethyl, 2-methyl-	14676-29-0	0.053	0.084
132	Mixture		0.0033	0.0067
133	Octane, 3-methyl-	2216-33-3	0.0046	0.0091
134	Cyclooctane, 1,4-dimethyl-, cis-	13151-99-0	0.039	0.008
135	3-Heptanone, 6-methyl-	624-42-0	0.0082	0.0163
136	2-Heptanone, 6-methyl-	928-68-7	0.36	0.05
137	Benzene, propyl-	103-65-1	0.0041	0.0082
138	Nonane, 4-methyl-	17301-94-9	0.067	0.005
139	C10-Alkene		0.076	0.004
140	Alkanone		0.059	0.005
141	C10-Alkene		0.031	0.062
142	Octane, 3,5-dimethyl-	15869-93-9	0.078	0.090
143	Unknown		0.013	0.027
144	Alkene		0.026	0.052
145	4-Octanone	589-63-9	0.031	0.004
146	Cyclopentane,1-methyl-3-(2-methylpropyl	29053-04-1	0.022	0.005
147	Phenol	108-95-2	0.046	0.013
148	Cyclotetrasiloxane, octamethyl-	556-67-2	0.070	0.014
149	Cyclopentane, 1,1,3,4-tetramethyl-cis,	53907-60-1	0.0054	0.0108
150	Decane	124-18-5	0.25	0.02
151	Mixture		0.018	0.002
152	Benzene, 2-propenyl- and others		0.0051	0.0101
153	Alkyl-Cyclohexane		0.019	0.005
154	C11-Alkane		0.012	0.002
155	C6-Cyclopentane		0.016	0.002

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
156	Nonane, 2,6-dimethyl-	17302-28-2	0.19	0.01
157	Decane, 2-methyl-	6975-98-0	0.027	0.005
158	1-Hexanol, 2-ethyl-	104-76-7	0.019	0.003
159	Mixture		0.025	0.004
160	Nonane, 3,7-dimethyl-	17302-32-8	0.081	0.017
161	Mixture		0.037	0.043
162	Cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.041	0.004
163	Alkanone		0.053	0.029
164	C12-Alkene		0.13	0.01
165	Decane, 4-methyl-	2847-72-5	0.053	0.007
166	C10-Alkanone		0.19	0.01
167	Naphthalene, decahydro-, trans	493-02-7	0.15	0.01
168	Ethanone, 1-phenyl-	98-86-2	0.014	0.028
169	Phenol, 2-methyl- and others	95-48-7	0.015	0.030
170	alkyl-nitrile		0.017	0.034
171	5-Nonanone	502-56-7	0.0073	0.0084
172	Cyclohexane, 1,2-diethyl-1-methyl-	61141-79-5	0.022	0.026
173	C5-Cyclohexane		0.16	0.05
174	2-Nonanone	821-55-6	0.13	0.04
175	Undecane	1120-21-4	0.61	0.03
176	Cyclopentane, 1-methyl-2-(2-propenyl)-trans	50746-53-7	0.0085	0.0170
177	Octane, 6-ethyl-2-methyl-	62016-19-7	0.16	0.02
178	Undecane, 4-methyl-	2980-69-0	0.020	0.041
179	Octane, 2,5,6-trimethyl-	62016-14-2	0.0073	0.0147
180	C11-Alkane		0.0063	0.0127
181	Undecane, 5-methyl-	1632-70-8	0.11	0.07
182	C12-Alkane		0.058	0.039
183	Undecane, 2-methyl-	7045-71-8	0.30	0.01
184	C12-Alkene		0.0085	0.0170
185	Cyclopropane, 1-ethyl-2-heptyl-	74663-86-8	0.059	0.008
186	Cyclohexane, pentyl-	4292-92-6	0.035	0.069
187	Cyclohexanone, 5-methyl-2-(1-methylethy	15932-80-6	0.22	0.15

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
188	6-Methylundecane	17302-33-9	0.34	0.01
189	Undecane, 4-methyl-	2980-69-0	0.15	0.01
190	Undecane, 2-methyl-	7045-71-8	0.29	0.02
191	Undecane, 3-methyl or C12-alkane	1002-43-3	0.15	0.02
192	Cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.075	0.050
193	Undecane, 2,6-dimethyl-	17301-23-4	0.24	0.03
194	Dodecane, 4-methyl-	6117-97-1	0.060	0.041
195	Undecane, 2,10-dimethyl-	17301-27-8	0.15	0.02
196	Dodecane, 4,6-dimethyl-	61141-72-8	0.0081	0.0162
197	Tridecane, 2-methyl-	1560-96-9	0.11	0.08
198	Tridecane, 3-methyl-	6418-41-3	0.080	0.055
199	Tetradecane	629-59-4	0.23	0.17
200	Tridecane, 4,8-dimethyl-	55030-62-1	0.018	0.021
201	Mixture		0.024	0.016
202	C14-Alkene		0.016	0.032
203	Tetradecane, 4-ethyl-	55045-14-2	0.0089	0.0179
204	C15-Alkane		0.066	0.005
205	C15-Alkane		0.049	0.002
206	3-Hexadecene, (Z)-	34303-81-6	0.011	0.021
207	Pentadecane	629-62-9	0.25	0.16
208	Mixture		0.017	0.003
209	Tetradecane, 2,6,10-trimethyl-	14905-56-7	0.032	0.002
210	Dodecane, 2-methyl-6-propyl-	55045-08-4	0.040	0.003
211	Decane, 3-cyclohexyl-, 3-cyclohexyl-	13151-74-1	0.046	0.002
212	Alkanone		0.025	0.004
213	Hexadecane	544-76-3	0.11	0.02
214	Tridecane, 5-propyl-	55045-11-9	0.028	0.003
215	Alkane		0.0013	0.0027
216	Alkanone		0.0034	0.0040
217	Heptadecane	629-78-7	0.014	0.003
218	Pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.014	0.003
219	Tetradecanoic acid	544-63-8	0.010	0.006

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
220	Octadecane	593-45-3	0.0010	0.0020
221	1,1'-Biphenyl, 2,6-dichloro and siloxane		0.0013	0.0027
222	Benzenesulfonamide, N-butyl-	3622-84-2	0.042	0.008
223	Alkane		0.0014	0.0027
224	9-Hexadecenoic acid	2091-29-4	0.0023	0.0046
225	Hexadecanoic acid	57-10-3	0.014	0.012
226	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.012	0.005
227	Alkane		0.0043	0.0086
Sum of tentatively identified compounds:			25.72	

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero, values listed are estimates.

Table 4-8
Tank BY-104 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	1-Butene	106-98-9	0.66	0.77
20	1-Pentene, 4-methyl-	691-37-2	0.36	0.07
3	1-Propene, 2-methyl-	115-11-7	0.12	0.08
4	1-Propene, 2-methyl-	115-11-7	0.26	0.18
79	1-Pentene, 3,4-dimethyl-	7385-78-6	0.063	0.012
6	1-Butene, 3-methyl-	563-45-1	0.083	0.096
24	1-Hexene	592-41-6	0.015	0.030
158	1-Hexanol, 2-ethyl-	104-76-7	0.019	0.003
28	1-Hexene	592-41-6	0.49	0.10
27	1-Pentene, 2-methyl-	763-29-1	0.22	0.02
221	1,1'-Biphenyl, 2,6-dichloro and siloxane		0.0013	0.0027
42	1,3-Pentadiene, 2-methyl-	1118-58-7	0.25	0.05
17	1,3-Butadiene, 2-methyl-	78-79-5	0.12	0.03
19	1,3-Butadiene, 2-methyl-	78-79-5	0.035	0.041
87	1,4-Hexadiene, 4-methyl-	1116-90-1	0.0086	0.0172
43	1,4-Hexadiene	592-45-0	0.14	0.03
45	1,4-Hexadiene and siloxane	592-45-0	0.017	0.034
54	1,4-Hexadiene	592-45-0	0.012	0.015
47	1,5-Hexadiene	592-42-7	0.12	0.04
13	2-Propanol	67-63-0	0.14	0.27
14	2-Pentene, (Z)	627-20-3	0.095	0.015
88	2-Hexanone, 5-methyl-	110-12-3	0.045	0.007
174	2-Nonanone	821-55-6	0.13	0.04
109	2-Hexanone, 4-methyl-	105-42-0	0.14	0.10
60	2-Heptene	592-77-8	0.046	0.015
91	2-Ethyl-5-methylfuran	1703-52-2	0.012	0.025
99	2-Hexenal	505-57-7	0.0064	0.0127
64	2-Heptene (E)	592-77-8	0.034	0.007
56	2-Propenal, 2-methyl-	78-85-3	0.049	0.010

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
30	2-Butanone	78-93-3	1.4	0.6
5	2-Butene	107-01-7	0.089	0.060
32	2-Hexene, (E)	4050-45-7	0.090	0.004
33	2-Butene, 2,3-dimethyl-	563-79-1	0.12	0.03
34	2-Butanol and others		0.030	0.061
35	2-Propanol	67-63-0	0.063	0.073
8	2-Propanol and others		0.14	0.27
93	2-Hexanal	66-25-1	0.0066	0.0133
76	2-Pentanone, 3-methyl-	565-61-7	0.032	0.026
39	2-Propanol	67-63-0	0.46	0.07
71	2-Pentanol, 2-methyl-	590-36-3	0.050	0.005
130	2-Heptanone, 4-methyl-	6137-06-0	0.026	0.030
50	2-Butanone, 3-methyl-	563-80-4	0.052	0.012
136	2-Heptanone, 6-methyl-	928-68-7	0.36	0.05
44	2-Butanol, 2-methyl-	75-85-4	0.035	0.044
61	2,3-Pentanedione	600-14-6	0.018	0.036
118	3-Heptanone	106-35-4	0.14	0.08
206	3-Hexadecene, (Z)-	34303-81-6	0.011	0.021
63	3-Pentanone, 2-methyl-	565-69-5	0.052	0.037
58	3-Heptene, (E)	14686-14-7	0.018	0.014
94	3-Octene, (E)	14919-01-8	0.13	0.19
135	3-Heptanone, 6-methyl-	624-42-0	0.0082	0.0163
75	3-Pentanone, 2-methyl-	565-69-5	0.0081	0.0162
103	3-Penten-1-ol and others		0.019	0.013
89	3-Hexanone	589-38-8	0.14	0.02
55	3-Buten-2-one, 3-methyl-	814-78-8	0.019	0.038
29	3-Buten-2-one	78-94-4	0.16	0.02
145	4-Octanone	589-63-9	0.031	0.004
82	4-Pentenol, 2-ethyl-		0.018	0.035
116	4-Octen-3-one	14129-48-7	0.0045	0.0089
171	5-Nonanone	502-56-7	0.0073	0.0084
188	6-Methylundecane	17302-33-9	0.34	0.01

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
224	9-Hexadecenoic acid	2091-29-4	0.0023	0.0046
96	Acetic acid, butyl ester	123-86-4	0.023	0.005
69	Alkane and others		0.0070	0.0141
80	Alkane and siloxane		0.059	0.119
215	Alkane		0.0013	0.0027
223	Alkane		0.0014	0.0027
227	Alkane		0.0043	0.0086
59	Alkanol		0.030	0.005
86	Alkanol		0.023	0.034
92	Alkanol		0.0065	0.0130
128	Alkanol		0.0078	0.0091
140	Alkanone		0.059	0.005
163	Alkanone		0.053	0.029
212	Alkanone		0.025	0.004
216	Alkanone		0.0034	0.0040
68	Alkene and others		0.033	0.024
85	Alkene		0.32	0.04
144	Alkene		0.026	0.052
170	alkyl-nitrile		0.017	0.034
153	Alkyl-Cyclohexane		0.019	0.005
115	Benzene, 1,2-dimethyl-	95-47-6	0.039	0.079
120	Benzene, 1,2-dimethyl-	95-47-6	0.029	0.030
137	Benzene, propyl-	103-65-1	0.0041	0.0082
152	Benzene, 2-propenyl- and others		0.0051	0.0101
222	Benzenesulfonamide, N-butyl-	3622-84-2	0.042	0.008
2	Butane	106-97-8	0.73	0.85
7	Butane, 2-methyl-	78-78-4	0.90	0.60
78	Butane, 2,2,3,3-tetramethyl-	594-82-1	0.017	0.034
117	Butane, 1,1'-oxybis-	142-96-1	0.037	0.028
166	C10-Alkanone		0.19	0.01
139	C10-Alkene		0.076	0.004
141	C10-Alkene		0.031	0.062

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
154	C11-Alkane		0.012	0.002
180	C11-Alkane		0.0063	0.0127
164	C12-Alkene		0.13	0.01
184	C12-Alkene		0.0085	0.0170
182	C12-Alkane		0.058	0.039
202	C14-Alkene		0.016	0.032
205	C15-Alkane		0.049	0.002
204	C15-Alkane		0.066	0.005
11	C5-Alkane		1.0	2.0
173	C5-Cyclohexane		0.16	0.05
155	C6-Cyclopentane		0.016	0.002
23	C6-Alkene		0.36	0.18
25	C6-Alkene		0.012	0.024
105	C7-Alkanone		0.0052	0.0104
90	C7-Alkene		0.0099	0.0199
46	C7-Alkene		0.041	0.048
110	C7-Alkanone		0.050	0.100
52	C8-Alkene		0.017	0.012
83	C8-Alkane		0.077	0.153
125	C8-Alkanone		0.049	0.003
114	C9-Alkane		0.17	0.06
21	Cyclobutanone	1191-95-3	0.15	0.04
48	Cyclohexane	110-82-7	0.054	0.037
65	Cyclohexane, methyl-	108-87-2	0.17	0.02
104	Cyclohexane, ethyl-	1678-91-7	0.042	0.004
106	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.061	0.018
111	Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)-	1795-27-3	0.0056	0.0112
124	Cyclohexane, 1-ethyl-4-methyl-trans-	6236-88-0	0.0025	0.0051
186	Cyclohexane, pentyl-	4292-92-6	0.035	0.069
192	Cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.075	0.050
122	Cyclohexane, 1-ethyl-4-methyl,cis	4926-78-7	0.0019	0.0039

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
172	Cyclohexane, 1,2-diethyl-1-methyl-	61141-79-5	0.022	0.026
187	Cyclohexanone, 5-methyl-2-(1-methylethy	15932-80-6	0.22	0.15
134	Cyclooctane, 1,4-dimethyl-, cis-	13151-99-0	0.039	0.008
15	Cyclopentane	287-92-3	0.16	0.11
57	Cyclopentane, 1,2-dimethyl-	2452-99-5	0.050	0.005
70	Cyclopentane, ethyl-	1640-89-7	0.011	0.022
72	Cyclopentane, 1,2,4-trimethyl-, (1.alpha.,2.alpha.,4.beta.)-	4850-28-6	0.022	0.015
149	Cyclopentane, 1,1,3,4-tetramethyl-cis,	53907-60-1	0.0054	0.0108
162	Cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.041	0.004
176	Cyclopentane, 1-methyl-2-(2-propenyl)-trans	50746-53-7	0.0085	0.0170
146	Cyclopentane, 1-methyl-3-(2-methylpropyl	29053-04-1	0.022	0.005
10	Cyclopropane, ethyl-	1191-96-4	0.76	0.33
16	Cyclopropane, 1,1-dimethyl-	1630-94-0	0.091	0.063
36	Cyclopropane, propyl-	2415-72-7	0.11	0.02
38	Cyclopropane, (1-methylethyl)-	3638-35-5	0.29	0.06
185	Cyclopropane, 1-ethyl-2-heptyl-	74663-86-8	0.059	0.008
148	Cyclotetrasiloxane, octamethyl-	556-67-2	0.070	0.014
150	Decane	124-18-5	0.25	0.02
157	Decane, 2-methyl-	6975-98-0	0.027	0.005
165	Decane, 4-methyl-	2847-72-5	0.053	0.007
211	Decane, 3-cyclohexyl-, 3-cyclohexyl-	13151-74-1	0.046	0.002
194	Dodecane, 4-methyl-	6117-97-1	0.060	0.041
196	Dodecane, 4,6-dimethyl-	61141-72-8	0.0081	0.0162
210	Dodecane, 2-methyl-6-propyl-	55045-08-4	0.040	0.003
168	Ethanone, 1-phenyl-	98-86-2	0.014	0.028
53	Formic acid, butyl ester	592-84-7	0.0075	0.0151
31	Furan, 2-methyl-	534-22-5	0.019	0.039
62	Furan, 2,5-dimethyl-	625-86-5	0.0097	0.0193
217	Heptadecane	629-78-7	0.014	0.003
81	Heptane, 2-methyl-	592-27-8	0.15	0.30
84	Heptane, 4-methyl-	589-53-7	0.12	0.02

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
101	Heptane, 2,6-dimethyl-	1072-05-5	0.13	0.02
112	Heptane, 2,3-dimethyl-	3074-71-3	0.036	0.008
113	Heptane, 2,6-dimethyl-	1072-05-5	0.045	0.031
131	Heptane, 3-ethyl, 2-methyl-	14676-29-0	0.053	0.084
213	Hexadecane	544-76-3	0.11	0.02
225	Hexadecanoic acid	57-10-3	0.014	0.012
226	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.012	0.005
97	Hexamethylcyclotrisiloxane	541-05-9	0.014	0.016
51	Hexane, 2-methyl-	591-76-4	0.17	0.01
9	Methane, trichlorofluoro-	75-69-4	0.58	0.39
12	Mixture of pentene and pentyne		0.29	0.18
18	Mixture of 2-propanenitrile & C6-Alkane		0.10	0.02
37	Mixture		0.11	0.01
100	Mixture		0.0062	0.0123
107	Mixture		0.086	0.020
108	Mixture		0.076	0.008
126	Mixture		0.010	0.001
127	Mixture		0.047	0.008
132	Mixture		0.0033	0.0067
151	Mixture		0.018	0.002
159	Mixture		0.025	0.004
161	Mixture		0.037	0.043
201	Mixture		0.024	0.016
208	Mixture		0.017	0.003
167	Naphthalene, decahydro-, trans	493-02-7	0.15	0.01
66	Nitric Acid, ethyl ester	625-58-1	0.0046	0.0092
138	Nonane, 4-methyl-	17301-94-9	0.067	0.005
156	Nonane, 2,6-dimethyl-	17302-28-2	0.19	0.01
160	Nonane, 3,7-dimethyl-	17302-32-8	0.081	0.017
220	Octadecane	593-45-3	0.0010	0.0020
129	Octane, 2,6-dimethyl-	2051-30-1	0.11	0.03
133	Octane, 3-methyl-	2216-33-3	0.0046	0.0091

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
142	Octane, 3,5-dimethyl-	15869-93-9	0.078	0.090
177	Octane, 6-ethyl-2-methyl-	62016-19-7	0.16	0.02
179	Octane,2,5,6-trimethyl-	62016-14-2	0.0073	0.0147
207	Pentadecane	629-62-9	0.25	0.16
218	Pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.014	0.003
49	Pentanal	110-62-3	0.021	0.042
73	Pentanal, 2-methyl-	123-15-9	0.23	0.03
22	Pentane, 2-methyl-	107-83-5	2.0	0.3
26	Pentane, 3-methyl-	96-14-0	0.48	0.11
121	Pentane, 1-methoxy-	628-80-8	0.037	0.006
102	Phenol, 2-methyl-	95-48-7	0.010	0.020
147	Phenol	108-95-2	0.046	0.013
169	Phenol, 2-methyl- and others	95-48-7	0.015	0.030
40	Propanenitrile, 2-methyl-	78-82-0	0.015	0.031
98	Pyridine, 4-methyl-	108-89-4	0.0046	0.0091
74	Siloxane and others		0.045	0.030
119	Styrene	100-42-5	0.026	0.009
95	Tetrachloroethylene	127-18-4	0.012	0.014
199	Tetradecane	629-59-4	0.23	0.17
203	Tetradecane, 4-ethyl-	55045-14-2	0.0089	0.0179
209	Tetradecane, 2,6,10-trimethyl-	14905-56-7	0.032	0.002
219	Tetradecanoic acid	544-63-8	0.010	0.006
41	Tetrahydrofuran	109-99-9	0.79	0.11
123	Tetramethylcyclohexane		0.0051	0.0060
197	Tridecane, 2-methyl-	1560-96-9	0.11	0.08
198	Tridecane, 3-methyl-	6418-41-3	0.080	0.055
200	Tridecane, 4,8-dimethyl-	55030-62-1	0.018	0.021
214	Tridecane, 5-propyl-	55045-11-9	0.028	0.003
175	Undecane	1120-21-4	0.61	0.03
178	Undecane, 4-methyl-	2980-69-0	0.020	0.041
181	Undecane, 5-methyl-	1632-70-8	0.11	0.07
183	Undecane, 2-methyl-	7045-71-8	0.30	0.01

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
189	Undecane, 4-methyl-	2980-69-0	0.15	0.01
190	Undecane, 2-methyl-	7045-71-8	0.29	0.02
191	Undecane, 3-methyl or C12-alkane	1002-43-3	0.15	0.02
193	Undecane, 2,6-dimethyl-	17301-23-4	0.24	0.03
195	Undecane, 2,10-dimethyl-	17301-27-8	0.15	0.02
67	Unknown		0.017	0.020
77	Unknown		0.014	0.028
143	Unknown		0.013	0.027

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero, values listed are estimates.

Table 4-9
Tank BY-104 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)
22	Pentane, 2-methyl-	107-83-5	2.0	0.3
30	2-Butanone	78-93-3	1.4	0.6
11	C5-Alkane		1.0	2.0
7	Butane, 2-methyl-	78-78-4	0.90	0.60
41	Tetrahydrofuran	109-99-9	0.79	0.11
10	Cyclopropane, ethyl-	1191-96-4	0.76	0.33
2	Butane	106-97-8	0.73	0.85
1	1-Butene	106-98-9	0.66	0.77
175	Undecane	1120-21-4	0.61	0.03
9	Methane, trichlorofluoro-	75-69-4	0.58	0.39
28	1-Hexene	592-41-6	0.49	0.10
26	Pentane, 3-methyl-	96-14-0	0.48	0.11
39	2-Propanol	67-63-0	0.46	0.07
23	C6-Alkene		0.36	0.18
136	2-Heptanone, 6-methyl-	928-68-7	0.36	0.05
20	1-Pentene, 4-methyl-	691-37-2	0.36	0.07
188	6-Methylundecane	17302-33-9	0.34	0.01
85	Alkene		0.32	0.04
183	Undecane, 2-methyl-	7045-71-8	0.30	0.01
12	Mixture of pentene and pentyne		0.29	0.18
190	Undecane, 2-methyl-	7045-71-8	0.29	0.02
38	Cyclopropane, (1-methylethyl)-	3638-35-5	0.29	0.06
4	1-Propene, 2-methyl-	115-11-7	0.26	0.18
207	Pentadecane	629-62-9	0.25	0.16
42	1,3-Pentadiene, 2-methyl-	1118-58-7	0.25	0.05
150	Decane	124-18-5	0.25	0.02
193	Undecane, 2,6-dimethyl-	17301-23-4	0.24	0.03
73	Pentanal, 2-methyl-	123-15-9	0.23	0.03
199	Tetradecane	629-59-4	0.23	0.17

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
187	Cyclohexanone, 5-methyl-2-(1-methylethy	15932-80-6	0.22	0.15
27	1-Pentene, 2-methyl-	763-29-1	0.22	0.02
166	C10-Alkanone		0.19	0.01
156	Nonane, 2,6-dimethyl-	17302-28-2	0.19	0.01
114	C9-Alkane		0.17	0.06
65	Cyclohexane, methyl-	108-87-2	0.17	0.02
51	Hexane, 2-methyl-	591-76-4	0.17	0.01
177	Octane, 6-ethyl-2-methyl-	62016-19-7	0.16	0.02
173	C5-Cyclohexane		0.16	0.05
15	Cyclopentane	287-92-3	0.16	0.11
29	3-Buten-2-one	78-94-4	0.16	0.02
191	Undecane, 3-methyl or C12-alkane	1002-43-3	0.15	0.02
195	Undecane, 2,10-dimethyl-	17301-27-8	0.15	0.02
21	Cyclobutanone	1191-95-3	0.15	0.04
81	Heptane, 2-methyl-	592-27-8	0.15	0.30
189	Undecane, 4-methyl-	2980-69-0	0.15	0.01
167	Naphthalene, decahydro-, trans	493-02-7	0.15	0.01
43	1,4-Hexadiene	592-45-0	0.14	0.03
118	3-Heptanone	106-35-4	0.14	0.08
13	2-Propanol	67-63-0	0.14	0.27
89	3-Hexanone	589-38-8	0.14	0.02
8	2-Propanol and others		0.14	0.27
109	2-Hexanone, 4-methyl-	105-42-0	0.14	0.10
94	3-Octene, (E)	14919-01-8	0.13	0.19
174	2-Nonanone	821-55-6	0.13	0.04
101	Heptane, 2,6-dimethyl-	1072-05-5	0.13	0.02
164	C12-Alkene		0.13	0.01
33	2-Butene, 2,3-dimethyl-	563-79-1	0.12	0.03
47	1,5-Hexadiene	592-42-7	0.12	0.04
3	1-Propene, 2-methyl-	115-11-7	0.12	0.08
17	1,3-Butadiene, 2-methyl-	78-79-5	0.12	0.03
84	Heptane, 4-methyl-	589-53-7	0.12	0.02

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
129	Octane, 2,6-dimethyl-	2051-30-1	0.11	0.03
213	Hexadecane	544-76-3	0.11	0.02
36	Cyclopropane, propyl-	2415-72-7	0.11	0.02
181	Undecane, 5-methyl-	1632-70-8	0.11	0.07
197	Tridecane, 2-methyl-	1560-96-9	0.11	0.08
37	Mixture		0.11	0.01
18	Mixture of 2-propanenitrile & C6-Alkane		0.10	0.02
14	2-Pentene, (Z)	627-20-3	0.095	0.015
16	Cyclopropane, 1,1-dimethyl-	1630-94-0	0.091	0.063
32	2-Hexene, (E)	4050-45-7	0.090	0.004
5	2-Butene	107-01-7	0.089	0.060
107	Mixture		0.086	0.020
6	1-Butene, 3-methyl-	563-45-1	0.083	0.096
160	Nonane, 3,7-dimethyl-	17302-32-8	0.081	0.017
198	Tridecane, 3-methyl-	6418-41-3	0.080	0.055
142	Octane, 3,5-dimethyl-	15869-93-9	0.078	0.090
83	C8-Alkane		0.077	0.153
108	Mixture		0.076	0.008
139	C10-Alkene		0.076	0.004
192	Cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.075	0.050
148	Cyclotetrasiloxane, octamethyl-	556-67-2	0.070	0.014
138	Nonane, 4-methyl-	17301-94-9	0.067	0.005
204	C15-Alkane		0.066	0.005
79	1-Pentene, 3,4-dimethyl-	7385-78-6	0.063	0.012
35	2-Propanol	67-63-0	0.063	0.073
106	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.061	0.018
194	Dodecane, 4-methyl-	6117-97-1	0.060	0.041
80	Alkane and siloxane		0.059	0.119
140	Alkanone		0.059	0.005
185	Cyclopropane, 1-ethyl-2-heptyl-	74663-86-8	0.059	0.008
182	C12-Alkane		0.058	0.039
48	Cyclohexane	110-82-7	0.054	0.037

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
165	Decane, 4-methyl-	2847-72-5	0.053	0.007
131	Heptane, 3-ethyl, 2-methyl-	14676-29-0	0.053	0.084
163	Alkanone		0.053	0.029
63	3-Pentanone, 2-methyl-	565-69-5	0.052	0.037
50	2-Butanone, 3-methyl-	563-80-4	0.052	0.012
110	C7-Alkanone		0.050	0.100
57	Cyclopentane, 1,2-dimethyl-	2452-99-5	0.050	0.005
71	2-Pentanol, 2-methyl-	590-36-3	0.050	0.005
205	C15-Alkane		0.049	0.002
125	C8-Alkanone		0.049	0.003
56	2-Propenal, 2-methyl-	78-85-3	0.049	0.010
127	Mixture		0.047	0.008
211	Decane, 3-cyclohexyl-, 3-cyclohexyl-	13151-74-1	0.046	0.002
147	Phenol	108-95-2	0.046	0.013
60	2-Heptene	592-77-8	0.046	0.015
113	Heptane, 2,6-dimethyl-	1072-05-5	0.045	0.031
74	Siloxane and others		0.045	0.030
88	2-Hexanone, 5-methyl-	110-12-3	0.045	0.007
104	Cyclohexane, ethyl-	1678-91-7	0.042	0.004
222	Benzenesulfonamide, N-butyl-	3622-84-2	0.042	0.008
46	C7-Alkene		0.041	0.048
162	Cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.041	0.004
210	Dodecane, 2-methyl-6-propyl-	55045-08-4	0.040	0.003
115	Benzene, 1,2-dimethyl-	95-47-6	0.039	0.079
134	Cyclooctane, 1,4-dimethyl-, cis-	13151-99-0	0.039	0.008
117	Butane, 1,1'-oxybis-	142-96-1	0.037	0.028
161	Mixture		0.037	0.043
121	Pentane, 1-methoxy-	628-80-8	0.037	0.006
112	Heptane, 2,3-dimethyl-	3074-71-3	0.036	0.008
44	2-Butanol, 2-methyl-	75-85-4	0.035	0.044
19	1,3-Butadiene, 2-methyl-	78-79-5	0.035	0.041
186	Cyclohexane, pentyl-	4292-92-6	0.035	0.069

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
64	2-Heptene (E)	592-77-8	0.034	0.007
68	Alkene and others		0.033	0.024
209	Tetradecane, 2,6,10-trimethyl-	14905-56-7	0.032	0.002
76	2-Pentanone, 3-methyl-	565-61-7	0.032	0.026
145	4-Octanone	589-63-9	0.031	0.004
141	C10-Alkene		0.031	0.062
34	2-Butanol and others		0.030	0.061
59	Alkanol		0.030	0.005
120	Benzene, 1,2-dimethyl-	95-47-6	0.029	0.030
214	Tridecane, 5-propyl-	55045-11-9	0.028	0.003
157	Decane, 2-methyl-	6975-98-0	0.027	0.005
119	Styrene	100-42-5	0.026	0.009
130	2-Heptanone,4-methyl-	6137-06-0	0.026	0.030
144	Alkene		0.026	0.052
212	Alkanone		0.025	0.004
159	Mixture		0.025	0.004
201	Mixture		0.024	0.016
86	Alkanol		0.023	0.034
96	Acetic acid, butyl ester	123-86-4	0.023	0.005
172	Cyclohexane,1,2-diethyl-1-methyl-	61141-79-5	0.022	0.026
146	Cyclopentane,1-methyl-3-(2-methylpropyl	29053-04-1	0.022	0.005
72	Cyclopentane, 1,2,4-trimethyl-, (1.alpha.,2.alpha.,4.beta.)-	4850-28-6	0.022	0.015
49	Pentanal	110-62-3	0.021	0.042
178	Undecane, 4-methyl-	2980-69-0	0.020	0.041
103	3-Penten-1-ol and others		0.019	0.013
31	Furan, 2-methyl-	534-22-5	0.019	0.039
55	3-Buten-2-one, 3-methyl-	814-78-8	0.019	0.038
153	Alkyl-Cyclohexane		0.019	0.005
158	1-Hexanol, 2-ethyl-	104-76-7	0.019	0.003
58	3-Heptene, (E)	14686-14-7	0.018	0.014
151	Mixture		0.018	0.002

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
82	4-Pentenal, 2-ethyl-		0.018	0.035
200	Tridecane, 4,8-dimethyl-	55030-62-1	0.018	0.021
61	2,3-Pentanedione	600-14-6	0.018	0.036
45	1,4-Hexadiene and siloxane	592-45-0	0.017	0.034
52	C8-Alkene		0.017	0.012
78	Butane, 2,2,3,3-tetramethyl-	594-82-1	0.017	0.034
208	Mixture		0.017	0.003
170	alkyl-nitrile		0.017	0.034
67	Unknown		0.017	0.020
155	C6-Cyclopentane		0.016	0.002
202	C14-Alkene		0.016	0.032
24	1-Hexene	592-41-6	0.015	0.030
169	Phenol, 2-methyl- and others	95-48-7	0.015	0.030
40	Propanenitrile, 2-methyl-	78-82-0	0.015	0.031
168	Ethanone, 1-phenyl-	98-86-2	0.014	0.028
97	Hexamethylcyclotrisiloxane	541-05-9	0.014	0.016
77	Unknown		0.014	0.028
218	Pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.014	0.003
225	Hexadecanoic acid	57-10-3	0.014	0.012
217	Heptadecane	629-78-7	0.014	0.003
143	Unknown		0.013	0.027
154	C11-Alkane		0.012	0.002
25	C6-Alkene		0.012	0.024
54	1,4-Hexadiene	592-45-0	0.012	0.015
91	2-Ethyl-5-methylfuran	1703-52-2	0.012	0.025
226	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.012	0.005
95	Tetrachloroethylene	127-18-4	0.012	0.014
70	Cyclopentane, ethyl-	1640-89-7	0.011	0.022
206	3-Hexadecene, (Z)-	34303-81-6	0.011	0.021
219	Tetradecanoic acid	544-63-8	0.010	0.006
102	Phenol, 2-methyl-	95-48-7	0.010	0.020
126	Mixture		0.010	0.001

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
90	C7-Alkene		0.0099	0.0199
62	Furan, 2,5-dimethyl-	625-86-5	0.0097	0.0193
203	Tetradecane, 4-ethyl-	55045-14-2	0.0089	0.0179
87	1,4-Hexadiene, 4-methyl-	1116-90-1	0.0086	0.0172
184	C12-Alkene		0.0085	0.0170
176	Cyclopentane, 1-methyl-2-(2-propenyl)-trans	50746-53-7	0.0085	0.0170
135	3-Heptanone, 6-methyl-	624-42-0	0.0082	0.0163
196	Dodecane, 4,6-dimethyl-	61141-72-8	0.0081	0.0162
75	3-Pentanone, 2-methyl-	565-69-5	0.0081	0.0162
128	Alkanol		0.0078	0.0091
53	Formic acid, butyl ester	592-84-7	0.0075	0.0151
179	Octane, 2,5,6-trimethyl-	62016-14-2	0.0073	0.0147
171	5-Nonanone	502-56-7	0.0073	0.0084
69	Alkane and others		0.0070	0.0141
93	2-Hexanal	66-25-1	0.0066	0.0133
92	Alkanol		0.0065	0.0130
99	2-Hexenal	505-57-7	0.0064	0.0127
180	C11-Alkane		0.0063	0.0127
100	Mixture		0.0062	0.0123
111	Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)-	1795-27-3	0.0056	0.0112
149	Cyclopentane, 1,1,3,4-tetramethyl-cis,	53907-60-1	0.0054	0.0108
105	C7-Alkanone		0.0052	0.0104
152	Benzene, 2-propenyl- and others		0.0051	0.0101
123	Tetramethylcyclohexane		0.0051	0.0060
66	Nitric Acid, ethyl ester	625-58-1	0.0046	0.0092
133	Octane, 3-methyl-	2216-33-3	0.0046	0.0091
98	Pyridine, 4-methyl-	108-89-4	0.0046	0.0091
116	4-Octen-3-one	14129-48-7	0.0045	0.0089
227	Alkane		0.0043	0.0086
137	Benzene, propyl-	103-65-1	0.0041	0.0082
216	Alkanone		0.0034	0.0040

WHC-SD-WM-ER-418 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
132	Mixture		0.0033	0.0067
221	1,1'-Biphenyl, 2,6-dichloro and siloxane		0.0013	0.0027
124	Cyclohexane, 1-ethyl-4-methyl-trans-	6236-88-0	0.0025	0.0051
224	9-Hexadecenoic acid	2091-29-4	0.0023	0.0046
122	Cyclohexane, 1-ethyl-4-methyl, cis	4926-78-7	0.0019	0.0039
223	Alkane		0.0014	0.0027
215	Alkane		0.0013	0.0027
220	Octadecane	593-45-3	0.0010	0.0020

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero, values listed are estimates.