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TANK 241BY108 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
3/1994 & 10/1994

COMPLETE

ENGINEERING CHANGE NOTICE

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1. ECN (use no. from pg. 1)

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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	☐
Const. Spec.	☐	Engineering Procedure	☐	Human Factor Consideration	☐
Procurement Spec.	☐	Operating Instruction	☐	Computer Software	☐
Vendor Information	☐	Operating Procedure	☐	Electric Circuit Schedule	☐
OM Manual	☐	Operational Safety Requirement	☐	ICRS Procedure	☐
FSAR/SAR	☐	IEFD Drawing	☐	Process Control Manual/Plan	☐
Safety Equipment List	☐	Cell Arrangement Drawing	☐	Process Flow Chart	☐
Radiation Work Permit	☐	Essential Material Specification	☐	Purchase Requisition	☐
Environmental Impact Statement	☐	Fac. Proc. Samp. Schedule	☐	Tickler File	☐
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Characterization Results for Samples Collected in
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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-108 Headspace Gas and Vapor Characterization Results for Samples Collected in March 1994 and October 1994

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Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
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-108 Headspace Gas and Vapor Characterization Results

for Samples Collected in March 1994 and October 1994

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank BY-108 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 October 1994 sampling event, but also includes selected results of the March 1994 sampling event. The tank BY-108 headspace was sampled in March 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in October 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-108, 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-108 was vapor sampled in March 1994 using the *in situ* sampling (ISS) method, and again in October 1994 using the more robust vapor sampling system (VSS) method. Unfortunately, the ISS event sorbent trap samples were radiologically contaminated, and were never analyzed (Huckaby et al. 1995). Furthermore, there are 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 the total nonmethane organic carbon (TNMOC) measurement from the March 1994 ISS event are presented below, because this analysis was not performed on samples from the VSS event. All other results presented here are from the October 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-108 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-108 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank BY-108 is the second tank in a 3-tank cascade with tanks BY-107 and BY-109. It is connected to tanks BY-107 and BY-109 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade lines. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank BY-107 or BY-109 may be transferred to tank BY-108 (unless the cascade lines are obstructed).

The cascade of tanks BY-107, BY-108, and BY-109 is passively ventilated, which means that the tanks are allowed to exhale air, waste gases, and vapors as the barometric pressure falls, and inhale ambient air as the barometric pressure rises. Each of these tanks has its own filtered breather riser. Barometric pressure typically rises and falls on a diurnal cycle, producing an average daily exchange of air equal to about 0.46 % of each tank headspace (Huckaby 1994b). Changes in the concentrations of tank headspace constituents due to barometric pressure changes are consequently very slow.

2.0 SAMPLING EVENT

2.1 March 1994 *In Situ* Sampling Event

Tank BY-108 was sampled using ISS methods on March 24, 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 were collected from a point approximately 7.9 m below the top of the flange on riser 1, between 10:00 a.m. and 12:30 p.m. Though the sorbent traps were physically lowered down into the headspace to minimize loss of analytes through condensation, adsorption, or absorption by condensate, the SUMMA™ canister samples were collected using unheated transfer tubing.

Huckaby et al. (1995) give a general description of the ISS method and equipment. Pingel (1994a) provides field sampling information for the tank BY-108 March 1994 ISS event. In addition to the TNMOC measurement results presented below, McVeety et al. (1995a) and Rasmussen (1994a) provide other sample analysis results.

2.2 October 1994 Vapor Sampling System Sampling Event

Headspace gas and vapor samples were collected from tank BY-108 using the VSS on October 27, 1994 by WHC Sampling and Mobile Laboratories, (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-BY-108 Tank Characterization Plan* (Carpenter 1994). The tank headspace temperature was determined to be 25.7 °C. Air from the tank BY-108 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 1, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), 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 that accompanied the samples.

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 SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canisters were prepared and analyzed by PNL at PNL quality assurance impact level 2. McVeety et al. (1995b) describe sample preparation and analyses.

Analyses of inorganic vapor sorbent traps were completed within 20 days of sample collection, but analyses of SUMMATM canisters for inorganic compounds were not completed until 79 days after sample collection. Thus the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994) was satisfied for sorbent trap analyses, but not for SUMMATM sample inorganic analyses. It should be noted that these inorganic compounds (i.e., the permanent gases) would be expected to be very stable in SUMMATM canisters, and the results may not have been affected even though the 60-day holding time requirement was exceeded. The specified 60-day holding time limit was administratively chosen, because no holding time study has been performed to determine the stability of the inorganic compounds in SUMMATM canisters in the chemical matrix of tank air samples.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in the headspace of tank BY-108 reported to be 1040 ppmv, is the highest measured in any passively ventilated tank. Ammonia is thought to be a product of chemical and radiolytic waste degradation processes. It has been observed in virtually all other waste tanks that have been sampled, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 988 ppmv in tank U-106 (Klinger et al. 1995). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 1040 ppmv corresponds to less than 0.7 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The hydrogen concentration in tank BY-108 was determined to be 399 ppmv. In general, hydrogen is of concern as a fuel. The measured 399 ppmv of hydrogen in tank BY-108, however, represents only about 1 % of the LFL for hydrogen in air, and is not a flammability concern at this level.

Nitrous oxide was measured to be an average 641 ppmv in the 3 SUMMATM canister samples. This is higher than is typical of other passively ventilated tanks, but higher values have been reported. 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-108 headspace.

3.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 224 ppmv, is much lower than the normal ambient air concentration of about 350 to 400 ppmv. Carbon dioxide introduced by air exchange

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

with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial liquid, and condensate) in the tank. The 224 ppmv carbon dioxide concentration measured in tank BY-108 is within the normal range for the passively ventilated tank headspaces.

Carbon monoxide in the tank BY-108 headspace, measured to be < 76 ppmv, is not well characterized. The method quantitation limit, 76 ppmv, is above the highest waste tank carbon monoxide concentration measured to date ([26.7 ppmv] in tank C-103² Huckaby and Story 1994). Elevated carbon monoxide concentrations are thought to be due to the decomposition of organic waste in the tanks.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank BY-108 headspace were determined to be ≤ 0.03 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-108. Nitric oxide is commonly found at trace concentrations, presumably 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-108 headspace.

The water vapor concentration was measured by gravimetric analysis of 5 sorbent trap systems by PNL (McVeety et al. 1995b). The water vapor concentration of tank BY-108 was determined to be about 13.4 mg/L, at the tank headspace temperature of 25.7 °C and pressure of 984 mbar (737.7 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 18.5 mbar (13.9 torr), to a dew point of 16.3 °C, and to a relative humidity of 56 %. It was noted that less mass (water) had been trapped on each successive sample, yet no explanation has been offered for this observation. The relative standard deviation is also higher than typical for this measurement.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium ions produced by the waste combine 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 indicated the total activity of the sample to be below the method detection limit of 50 pCi/L (WHC 1995b).

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank BY-108 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. However, tank BY-108 headspace contains the highest ammonia concentration (1040 ppmv) measured in any passively ventilated tank headspace, and the hydrogen and nitrous oxide concentrations are both relatively high.

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

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are reasonable for the methods used at the measured concentrations. Relative standard deviations range from 8 % for ammonia to 38 % for carbon dioxide. The precision of reported inorganic gas and vapor measurements has generally been better than this for other tanks. The higher than typical relative standard deviations of the tank BY-108 measurements suggest minor problems with sample air transfer may have occurred, and/or analytical problems. The high ammonia and organic vapor concentrations in tank BY-108 may be partially responsible for the observed precision.

As discussed briefly in Section 1.4, it is possible that gases and vapors generated by the waste in tanks BY-107 and BY-109 could be transferred to tank BY-108 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 is mutual), or all constituents detected in one tank would be at or equal or higher concentrations in the other tank (if air tends to flow consistently from one to the other). Consideration of data in Table 3-2 indicates that the headspace compositions of tanks BY-107 and BY-108 are quite similar, but with generally lower concentrations being found in tank BY-107. The data are consistent with the premise that the cascade line between them plays a significant role in their ventilation, but does not prove this occurs. Results for tank BY-109 presented in Table 3-2 are from the September 1994 ISS event, and represent the only available data for that tank. The contrasting ammonia, hydrogen, and nitrous oxide concentrations in tanks BY-108 and BY-109 suggest tank BY-109 is not affecting the headspace of tank BY-108 significantly.

4.0 ORGANIC VAPORS

Organic vapors in the tank BY-108 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both laboratories used a gas chromatograph (GC) equipped with a mass spectrometer (MS) to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995) and McVeety et al. (1995b). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method (EPA 1988) was also performed by Oregon Graduate Institute of Science and Technology (OGIST) on samples collected in March 1994 by the ISS method (Rasmussen 1994a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-108. These results were produced at PNL quality assurance impact level 2. However, PNL analyses of organic vapors in SUMMA™ canisters were not completed until 87 days after sample collection, which exceeded the administratively chosen 60-day holding time allowed by the WHC quality assurance project plan (Keller 1994). No holding time study has been performed to determine the stability of the organic analytes in SUMMA™ canisters in the chemical matrix of tank air 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 outside the 95 % confidence interval for variance, suggesting that a bias may have been 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.

Listed in Table 4-1 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL. PNL performed analyses according to the EPA task order 14 (TO-14) methodology, but expanded the number of target analytes from 40 to 54 to include waste tank analytes of particular interest (EPA 1988, McVeety et al. 1995b). Of the original 40 TO-14 analytes, 32 were determined to be below the 0.002 ppmv quantitation limit of the analyses, and 3 of the 15 additional target analytes (ethanenitrile, propanenitrile, and n-butanenitrile) were below the 0.005 ppmv method quantitation limit. Averages reported are from analyses of 3 SUMMA™ canister samples.

ORNL positively identified 23 of 27 target analytes selected by WHC. Four target analytes (1,1-dichloroethene, n-heptanenitrile, tributyl phosphate and dibutyl butylphosphonate) were below their detection limits. Despite calibration of the instrument over about a 20-fold concentration range, the measured values for 9 of the 23 positively identified compounds were outside of the calibration range in at least 1 of the TST samples, and were not quantitated. The positively identified compounds, and their average concentrations from the analysis of 3 TSTs, are given in Tables 4-2, 4-3, and 4-4. Table 4-2 lists 12 quantitated compounds, Table 4-3 lists 8 compounds which were not quantitated in all 3 TST samples, and Table 4-4 lists 3 compounds for which the ORNL practical holding times were exceeded. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so no compound appears in more than 1 table. 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 butanal, 1-butanol, and 2-pentanone may have been affected by the 39-day period between sample collection and analysis (Jenkins 1995b). The concentration of these 3 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 butanal, 1-butanol, and 2-pentanone to be 1, 17, and 34 days respectively. It should be noted that the contractual holding time for the TST samples was 60 days.

The 11 target analytes common to both the ORNL and PNL analyses are listed with their measured concentrations in TST and SUMMA™ canister samples in Table 4-5. Comparison of the results from the 2 laboratories indicates the following:

- 1) An acceptable agreement for propanone and certain nonpolar analytes (i.e., n-hexane, n-heptane, toluene, and n-decane);
- 2) TST analyses indicate dichloromethane to be present at an average concentration of 1.2 ppmv, while none was detected in SUMMA™ canister samples;
- 3) TST analyses indicate ethanenitrile to be 0.94 ppmv, and n-butanenitrile to be 0.31 ppmv, while SUMMA™ analyses indicate each of these to be below their quantitation limit of 0.005 ppmv; and
- 4) the 2 methods disagree on the concentration of benzene by roughly a factor of 7.

The TST dichloromethane results are questionable. Individual TST sample results are relatively inconsistent; the individual results are 0.30, 2.3, and 1.0 ppmv, which average to 1.2 ppmv, have a standard deviation of 1.0 ppmv, and a relative standard deviation of 83 %.

Though the discrepancy between the TST and SUMMA™ sample nitrile results is currently not understood, the reported concentrations are not above action limits.

The most abundant analytes in Tables 4-1 through 4-4, neglecting the TST dichloromethane result, are 1-butanol, propanone, 1-propanol, n-hexane and tetrahydrofuran, each of which was measured to be above 1 ppmv. At the reported concentrations, the positively identified organic compounds do not individually or cumulatively represent a flammability hazard.

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 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 especially long (>200 compounds) and difficult to analyze, the list has been sorted alphanumerically by compound name in Table 4-8, and also in order of decreasing estimated concentrations Table 4-9. Numbers in the first columns of Tables 4-8 and 4-9 (Cmpd #) identify the location of the compound in Table 4-7.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and McVeety et al. (1995b), 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 split chromatographic peaks (e.g., Cmpd # 96 and 99 in Table 4-7). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

Concentrations given in Tables 4-6 through 4-9 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 collected on March 28, 1994 using the EPA TO-12 method (Rasmussen 1994a). Because OGIST did not have a WHC-approved quality assurance project plan in place when the samples were analyzed, this data should be considered secondary, and has been placed in brackets. The sample mean was [594 mg/m³], with a standard deviation of [14 mg/m³]. This value is very high compared to other waste tanks sampled to date. Only tank C-103, estimated to have [3,000 to 5,000 mg/m³] of TNMOC (Rasmussen and Einfeld 1994), is known to have a higher TNMOC concentration. For comparison, the TNMOC concentration in clean ambient air may range from 0.03 to 0.1 mg/m³, in polluted city air it may be 0.3 to 0.4 mg/m³.

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 the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane, n-tridecane, n-tetradecane, n-pentadecane) and methyl-substituted decahydronaphthalenes that were used as diluents for tributyl phosphate.

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

Neither TST nor SUMMA™ methods detected tributyl phosphate as a headspace constituent. The relatively high concentration of 1-butanol, however, is a strong indication that tributyl phosphate does exist in tank BY-108. That tributyl phosphate was not observed in the TST samples may be due to the facts that tributyl phosphate has a very low vapor pressure, and it has a tendency to be adsorbed by the high efficiency particulate air filters used during sampling to protect the samples from radiological particulate contamination.

In the semivolatile region of Tables 4-6 and 4-7, there are many branched alkanes. The abundance of these, as well as the decahydronaphthalenes, was also noted in tank BY-107, to which tank BY-108 is attached.

It is interesting to note that while there are many ketones identified (particularly 2-alkanones, of which the homologous series from propanone to 2-nonanone, and several others exist), there are only 3 aldehydes identified. In other NPH-rich tanks (notably sludge tanks in 241-C farm, e.g., C-108, C-109, C-111 and C-112) the aldehydes and ketones are found in comparable numbers. This may be indicative of the oxidative properties of the waste, as the oxidation of an aldehyde to an acid is chemically easier than the oxidation of ketones.

Similarly, tank BY-108 has fewer nitriles than other NPH-rich tanks. Camaioni et al. (1994) point out that the hydrolysis of aldoximes produces aldehydes, while the dehydration of aldoximes produces nitriles.

The observation that nitriles and aldehydes are found together in some tanks, and almost not at all in other NPH-rich tanks, appears to support the proposed aldoxime hydrolysis mechanism.

Though there is no toxicological or flammability hazard associated with the 0.13 ppmv of trichlorofluoromethane measured in tank BY-108 SUMMATM samples, its presence has been noted in many of the tanks sampled to date. The origin of trichlorofluoromethane in the waste tanks has not been established, however, it may be present from its use in urethane foam that were applied to concrete tank pits as a sealant.

The concentrations of organic vapors in tank BY-108 are generally very high compared to other passively ventilated tanks that have been sampled. It has the second highest known TNMOC concentration of any tank. In character the organic vapors in tank BY-108 are very similar to tank BY-107, to which it is connected via a cascade line. Because there are clearly a higher concentrations of organic vapors in tank BY-108 than in either tank BY-107 or tank BY-109 (Table 3-2), the origin of the organic vapors in tank BY-108 appears to be the waste stored in that tank.

5.0 SUMMARY

The tank BY-108 headspace was sampled in March 1994 and October 1994 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the March 1994 event and essentially all results from the October 1994 event have been reported. It was determined that no headspace constituents exceeded the flammability notification limits, but that ammonia, measured to be 1080 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-108 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	0.05	Organic vapors	4 tank air samples
		0.25	Organic vapors	4 tank air samples
		0.50	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 blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank BY-108 Inorganic Gas and Vapor Concentrations
Analyses by Pacific Northwest Laboratory

Compound	CAS ¹ Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	1040	80	8
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	224	86	38
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	< 76	--	--
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	399	78	20
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.03	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	641	109	17
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	18,800 (13.4 mg/L)	5,500 (3.9 mg/L)	29

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-107, BY-108, and BY-109 Headspace Constituents¹

Tank:	BY-107 ²	BY-108	BY-109 ³
Date sampled, (mo/day/yr)	10/26/94	10/27/94	9/22/94
Headspace temperature, (°C)	33.1	25.7	26.5
Ammonia, (ppmv)	972	1040	46
Hydrogen, (ppmv)	267	399	[56.3]
Carbon dioxide, (ppmv)	94	224	[126]
Carbon monoxide, (ppmv)	< 20	< 76	[0.41]
Nitric oxide, (ppmv)	0.13	≤ 0.03	≤ 0.04
Nitrogen dioxide, (ppmv)	≤ 0.02	≤ 0.02	≤ 0.03
Nitrous oxide, (ppmv)	621	641	[10.7]
Water vapor, (mg/m ³)	13.0	13.4	--
Water vapor, (% relative humidity)	36	56	--
Ethanenitrile (acetonitrile), (ppmv)	(2.2)	0.94	0.083
Propanone (acetone), (ppmv)	(3.9)	(8.2)	(0.39)
1-Butanol, (ppmv)	(7.9)	(58)	(0.79)
n-Dodecane, (ppmv)	0.21	0.80	(0.17)
n-Tridecane, (ppmv)	(0.26)	0.73	(0.27)
Total organic compounds ⁴ , (mg/m ³)	149.4	510	20.3

1 Inorganic gas or vapor results are from PNL except where noted for tank BY-109; 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 1995.

3 Results for BY-109 are from an ISS event, and presented for comparison only. Values in brackets are from OGIST (Rasmussen 1994b), and should be considered secondary data. Sample volume measurements used by PNL to calculate the ammonia, nitric oxide, and nitrogen dioxide concentrations (Pool et al. 1995), and by ORNL to calculate the organic vapor concentrations (Jenkins et al. 1994), may not be accurate to within 20 %. Pingel (1994b) describes the sampling event.

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

Table 4-1
Tank BY-108 Quantitatively Measured Organic Compound Average Concentrations --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Trichlorofluoromethane	75-69-4	0.128	0.064	5
2	Propanone (acetone)	67-64-1	4.4	0.5	11
3	1-Propanol	71-23-8	6.8	0.1	2
4	2-Butanone	78-93-3	0.54	0.33	60
5	n-Hexane	110-54-3	1.5	0.04	2
6	Benzene	71-43-2	0.025	0.001	2
7	4-Methyl-2-pentanone	108-10-1	0.037	0.001	2
8	Cyclohexane	110-82-7	0.14	0.005	3
9	n-Heptane	142-82-5	0.52	0.01	2
10	Tetrahydrofuran	109-99-9	1.29	0.02	2
11	Toluene	108-88-3	0.045	0.002	3
12	Ethylbenzene	100-41-4	0.185	0.0005	0.3
13	1,3-Dimethylbenzene (m-xylene) + 1,4-Dimethylbenzene (p-xylene) ⁴	108-38-3 106-42-3	0.077	0.003	4
14	o-Xylene	95-47-6	0.024	0.001	5
15	Cyclohexanone	108-94-1	0.010	0.002	16
16	n-Decane	124-18-5	0.090	0.002	3
17	Methane	74-82-8	< 61	--	--

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

Table 4-2
Tank BY-108 Quantitatively Measured Organic Compound Average Concentrations --
and Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.94	0.18	19
2	Dichloromethane	75-09-2	1.2	1.0	85
3	Butanenitrile	109-74-0	0.31	0.04	12
4	n-Heptane	142-82-5	0.89	0.03	3
5	2-Hexanone	591-78-6	0.16	0.02	15
6	n-Octane	111-65-9	0.33	0.08	23
7	2-Heptanone	110-43-0	0.14	0.03	19
8	n-Nonane	111-84-2	0.19	0.03	14
9	n-Decane	124-18-5	0.21	0.10	46
10	n-Undecane	1120-21-4	0.48	0.09	19
11	n-Dodecane	112-40-3	0.80	0.18	22
12	n-Tridecane	629-50-5	0.73	0.22	30

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 55 ml TST samples.

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

Table 4-3
Tank BY-108 Positively Identified Organic Compound Average Concentrations
and Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Propanone (acetone)	67-64-1	8.2	0.6	7
2	Propanenitrile	107-12-0	0.048	0.002	4
3	n-Hexane	110-54-3	2.3	0.1	3
4	Benzene	71-43-2	0.18	0.01	7
5	Toluene	108-88-3	0.10	0.02	17
6	Pentanenitrile	110-59-8	0.020	0.003	15
7	Hexanenitrile	628-73-9	0.022	0.002	9
8	2-Octanone	111-13-7	0.039	0.018	46

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, 55 ml TST samples.

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

Table 4-4
Tank BY-108 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Butanal ⁵	123-72-8	0.87	0.66	75
2	1-Butanol ⁶	71-36-3	58	5	8
3	2-Pentanone ⁵	107-87-9	0.46	0.07	16

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 55 ml TST samples.

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

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

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

Table 4-5
Tank BY-108 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 (%)
Ethanenitrile (acetonitrile)	75-05-8	0.94	< 0.005	> 198
Propanone (acetone) ⁵	67-64-1	8.2	4.4	60
Dichloromethane ⁵	75-09-2	1.2	< 0.005	> 198
Propanenitrile ⁵	107-12-0	0.048	< 0.005	> 162
n-Hexane	110-54-3	2.3	1.5	42
Benzene	71-43-2	0.18	0.025	> 151
Butanenitrile	109-74-0	0.31	< 0.005	> 194
n-Heptane	142-82-5	0.89	0.52	10
Toluene	108-88-3	0.10	0.045	76
Pentanenitrile ⁵	110-59-8	0.020	< 0.005	> 120
n-Decane	124-18-5	0.21	0.090	80

1 CAS = Chemical Abstract Service.

2 Average of 3, 55 ml TST samples.

3 Average of 3 samples from PNL.

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

5 Two or more of the sample results fell outside the calibration range.

Table 4-6
Tank BY-108 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propene	115-07-1	1.82	0.04
2	Propane	74-98-6	0.91	0.04
3	Cyclopropane	75-19-4	0.29	0.00
4	Isobutane	75-28-5	0.58	0.02
5	1-Butene	106-98-9	2.02	0.13
6	Butane	106-97-8	1.38	0.08
7	2-Methyl-1-Propene	115-11-7	0.22	0.00
8	Cyclobutane	287-23-0	0.40	0.01
9	Isopropyl Alcohol	67-63-0	0.22	0.01
10	1-Pentene	109-67-1	0.69	0.01
11	Pentane	109-66-0	1.37	0.09
12	4-Methyl-1-Pentene	691-37-2	0.53	0.04
13	2-Methylpentane	107-83-5	2.07	0.06
14	3-Methylpentane	96-14-0	0.40	0.01
15	1-Hexene	592-41-6	0.74	0.04
16	Methylcyclopentane	96-37-7	0.28	0.01
17	1-Butanol	71-36-3	12.60	0.75
18	2-Pentanone	107-87-9	1.66	0.07
19	3-Methylhexane	589-34-4	1.69	0.05
20	1-Heptene	592-76-7	1.14	0.11
21	Unknown C8 Alkene/Cycloalkane		0.34	0.03
22	Unknown C8 Alkane		1.26	0.03
23	2-Hexanone	591-78-6	0.66	0.04
24	Unknown C8 Alkene/Cycloalkane		0.21	0.01
25	1,2-Dimethylcyclohexane	583-57-3	0.25	0.01
26	1-Octene	111-66-0	0.31	0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Octane	111-65-9	1.36	0.05
28	2,6-dimethylheptane	1072-05-5	0.43	0.02
29	Unknown Alkene/Cycloalkane		0.41	0.02
30	2-Heptanone	110-43-0	0.32	0.02
31	Nonane	111-84-2	0.80	0.03
32	Unknown Ketone		0.75	0.04
33	Unknown C9 Alkene/Cycloalkane		0.27	0.02
34	Unknown C10 Alkane		0.25	0.01
35	2-Octanone	111-13-7	0.30	0.01
36	Unknown C10 Alkene/Cycloalkane		0.37	0.02
37	Unknown C10 Alkene/Cycloalkane		0.20	0.01
38	Unknown C10 Alkene/Cycloalkane		0.24	0.01
39	Unknown C11 Alkane		1.03	0.04
40	Unknown C11 Alkane		0.22	0.01
41	Unknown C10 Alkene/Cycloalkane		0.47	0.02
42	Unknown C11 Alkane		0.22	0.01
43	Unknown C11 Alkane		0.27	0.01
44	Unknown C11 Alkane		0.27	0.01
45	Decahydronaphthalene	91-17-8	0.32	0.01
46	1-Undecene	821-95-4	0.32	0.03
47	Undecane	1120-21-4	3.34	0.13
48	Unknown C11 Alkene/Cycloalkane		0.60	0.04
49	Unknown C12 Alkane		0.51	0.04
50	Unknown C12 Alkane		0.53	0.04
51	Naphthalene, decahydro-2-methyl-	2958-76-1	0.67	0.03
52	Unknown C11 Alkene/Cycloalkane		0.80	0.05
53	Unknown C12 Alkane		0.52	0.02
54	Decahydro-2-Methylnaphthalene	2958-76-1	0.30	0.01

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Unknown C12 Alkane		0.86	0.05
56	Unknown C12 Alkane		0.51	0.05
57	Unknown Alkyl Decahydronaphthalene		0.58	0.03
58	Dodecane	112-40-3	6.16	0.27
59	Unknown C12 Alkene/Cycloalkane		0.31	0.02
60	Decahydro-2,6-Dimethylnaphtalene	1618-22-0	0.58	0.03
61	2,6-Dimethylundecane	17301-23-4	4.18	0.22
62	Unknown C13 Alkane		0.46	0.06
63	Unknown Alkyl Decahydronaphthalene		0.57	0.04
64	Unknown C13 Alkene/Cycloalkane		2.36	0.19
65	Unknown Alkyl Decahydronaphthalene		0.71	0.07
66	Unknown C12 Alkane		0.98	0.12
67	Unknown Alkane		0.70	0.09
68	Unknown C14 Alkane		4.92	0.34
69	Unknown C13 Alkene/Cycloalkane		0.38	0.03
70	Tridecane	629-50-5	5.30	0.36
71	Unknown C13 Alkene/Cycloalkane		0.33	0.03
72	Unknown C14 Alkene/Cycloalkane		0.91	0.06
73	Unknown Alkane		1.11	0.14
74	Unknown C14 Alkene/Cycloalkane		0.25	0.02
75	Unknown C13 Alkene/Cycloalkane		0.99	0.10
76	2-Methyltridecane	1560-96-9	0.41	0.05
77	Unknown Alkane		0.23	0.03
78	2,6,10-Trimethyldodecane,	3891-98-3	2.43	0.24
79	Unknown C4 Alkyl Decahydronaphthalene		0.32	0.04
80	Tetradecane	629-59-4	1.95	0.25
81	Unknown C15 Alkene/Cycloalkane		0.41	0.14
Sum of tentatively identified compounds:			89.0	

1 CAS = Chemical Abstract Number.

2 Average of 3 samples, values listed are estimates.

Table 4-7
Tank BY-108 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	1-propene, 2-methyl-	115-11-7	1.6	1.5
2	1-propene, 2-methyl-	115-11-7	2.1	0.4
3	1-propene, 2-methyl-	115-11-7	0.48	0.84
4	1-butene, 3-methyl-	563-45-1	0.51	0.88
5	butane, 2-methyl-	78-78-4	7.9	0.8
6	methane, trichlorofluoro-	75-69-4	11.9	13.0
7	cyclopropane, ethyl-	1191-96-4	7.3	0.8
8	3-buten-1-ol	627-27-0	6.1	10.5
9	furan	110-00-9	0.55	0.96
10	oxirane, ethenyl-	930-22-3	0.8	1.4
11	2-propanol	67-63-0	5.3	1.6
12	2-pentene, (Z)-	627-20-3	0.88	0.76
13	cyclobutane, methyl-	598-61-8	0.92	0.80
14	1-pentene, 4-methyl-	691-37-2	2.5	0.3
15	pentane, 2-methyl-	107-83-5	15.1	0.9
16	1-propene, 2-fluoro-	1184-60-7	0.47	0.82
17	pentane, 3-methyl-	96-14-0	2.5	0.2
18	1-pentene, 2-methyl-	763-29-1	2.6	1.6
19	1-hexene	592-41-6	3.0	2.6
20	2-butanone	78-93-3	0.66	1.14
21	cyclopentane, methyl-	96-37-7	2.1	0.3
22	furan, tetrahydro-	109-99-9	8.5	2.0
23	1,3-pentadiene, 2-methyl-	1118-58-7	0.49	0.85
24	1-pentene, 3,4-dimethyl-	7385-78-6	0.59	1.02
25	1-hexene, 5-methyl-	3524-73-0	0.53	0.91
26	hexane, 2-methyl-	591-76-4	1.34	0.05

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	cyclopentane, 1,2-dimethyl-, trans-	822-50-4	0.324	0.305
28	cyclopropane, butyl-	930-57-4	2.5	0.3
29	2-heptene	592-77-8	0.16	0.28
30	cyclohexane, methyl-	108-87-2	1.13	0.06
31	mixture		0.14	0.24
32	propane, 2-nitro & others		0.14	0.23
33	1-heptene, 6-methyl-	5026-76-6	0.25	0.43
34	1-heptene, 3-methyl-	4810-09-7	0.52	0.46
35	heptane, 2,3,5-trimethyl-	20278-85-7	0.65	1.12
36	heptane, 2,3,6-trimethyl-	4032-93-3	1.26	1.10
37	1-octene	111-66-0	0.74	0.65
38	heptane, 3-methyl-	589-81-1	0.19	0.32
39	3-pentanol, 2-methyl- and others		0.11	0.19
40	cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.11	0.20
41	cyclopentane, 1,1,3-trimethyl-	4516-69-2	0.24	0.21
42	hexanal, 3-methyl-	19269-28-4	0.24	0.42
43	1-octene	111-66-0	0.18	0.31
44	2H-pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.81	0.72
45	1-octanol	111-87-5	0.12	0.20
46	hexamethylcyclotrisiloxane	541-05-9	0.13	0.22
47	heptane, 2,6-dimethyl-	1072-05-5	0.56	0.07
48	cyclohexane, ethyl-	1678-91-7	0.46	0.11
49	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.82	0.19
50	1-nonene	124-11-8	0.31	0.27
51	heptane, 2,3-dimethyl-	3074-71-3	0.09	0.16
52	benzene, ethyl and octane, 2-methyl-		0.54	0.05
53	benzene, 1,2-dimethyl-	95-47-6	0.40	0.69
54	benzene, 1,4-dimethyl-	106-42-3	0.35	0.61

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	heptane, 3,5-dimethyl-	926-82-9	0.073	0.126
56	octane, 3-methyl- and c2-benzene		0.43	0.74
57	butane, 1,1'-oxybis-	142-96-1	0.17	0.15
58	3-heptanone	106-35-4	0.68	0.10
59	benzene, 1,2-dimethyl-	95-47-6	0.38	0.06
60	mixture		0.069	0.119
61	cyclohexane, 1-ethyl-4-methyl-, trans-	6236-88-0	0.057	0.099
62	3,4-nonadiene	37050-03-6	0.48	0.14
63	heptane, 4-(1-methylethyl)-	52896-87-4	0.15	0.26
64	1-hexene, 4,5-dimethyl-	16106-59-5	0.11	0.20
65	4-nonyne	20184-91-2	0.13	0.23
66	2-heptanone, 6-methyl-	928-68-7	1.4	0.6
67	nonane, 4-methyl-	17301-94-9	0.57	0.25
68	cyclohexane, 1,1,4,4-tetramethyl-		0.41	0.12
69	2-octanol	123-96-6	0.40	0.20
70	3-buten-2-ol	598-32-3	4.8	3.9
71	2-heptyl furan		0.22	0.23
72	cyclohexane, 1-methyl-4-(1-methylethyl) & others		0.099	0.170
73	cyclopentanone,2-methyl-4-(2-methyl-propyl)	69770-96-3	0.16	0.27
74	cyclopentane,2-isopropyl-1,3-dimethyl-	32281-85-9	0.25	0.44
75	cyclohexane,1-methyl-4-(1-methylethyl)cis	6069-98-3	0.23	0.22
76	cyclopentane, 1-methyl-3-(2-methylpropyl)	29053-04-1	0.57	0.16
77	cyclotetrasiloxane, octamethyl-	556-67-2	1.1	0.9
78	cyclohexane, 1,5-diethyl-2,3-dimethyl-	74663-66-4	0.52	0.25
79	nonane, 2,6-dimethyl-	17302-28-2	2.2	1.1
80	octane, 6-ethyl-2-methyl-	62016-19-7	0.19	0.20
81	1,4-pentadiene, 2,3,4-trimethyl- & others		0.079	0.137
82	3-decyne	2384-85-2	0.51	0.17

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
83	cyclohexane, butyl-	1678-93-9	1.46	0.39
84	cyclohexane, 1-ethyl-4-methyl, cis	4926-78-7	0.16	0.14
85	cyclohexane, cyclopropyl-	32669-86-6	0.19	0.17
86	1-ethyl-2,2,6-trimethylcyclohexane		0.55	0.14
87	decane, 5-methyl-	13151-35-4	0.73	0.20
88	decane, 4-methyl-	2847-72-5	0.78	0.21
89	decane, 2-methyl-	6975-98-0	1.8	0.5
90	naphthalene, decahydro-, trans-	493-02-7	1.1	0.3
91	decane, 3-methyl-	13151-34-3	1.1	0.2
92	cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.47	0.12
93	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.37	0.10
94	cyclohexane, 1-(cyclohexylmethyl)-4-methyl-	66826-95-7	0.80	0.19
95	c5-cyclohexane		0.69	0.14
96	5-undecene	4941-53-1	1.0	0.3
97	2-nonanone and others	821-55-6	0.93	0.23
98	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.28	0.26
99	5-undecene	4941-53-1	0.49	0.13
100	1-undecene, 4-methyl-	74630-39-0	0.51	0.89
101	nonane, 3,7-dimethyl-	17302-32-8	0.80	1.39
102	undecane, 5-methyl-	1632-70-8	2.9	0.8
103	bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-		0.41	0.09
104	undecane, 4-methyl-	2980-69-0	0.36	0.09
105	naphthalene, decahydro-2-methyl-	2958-76-1	2.2	0.6
106	undecane, 3,8-dimethyl-	17301-30-3	1.0	0.9
107	undecane, 4,7-dimethyl-	17301-32-5	0.77	1.34
108	dimethyl-decahydronaphthalene		0.25	0.24
109	2-undecene, 8-methyl-	74630-44-7	0.38	0.12
110	1-dodecene	112-41-4	0.38	0.08

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
111	cyclopentane, (2-methylbutyl)-	53366-38-4	0.35	0.10
112	naphthalene, decahydro-2-methyl	2958-76-1	5.9	1.6
113	3-dodecene, (Z)-	7239-23-8	0.20	0.19
114	naphthalene, decahydro-2-methyl-	2958-76-1	0.21	0.19
115	6-methylundecane	17302-33-9	3.4	0.9
116	undecane, 4-methyl-	2980-69-0	1.9	0.5
117	undecane, 2-methyl-	7045-71-8	3.8	1.0
118	undecane, 2,3-dimethyl-	17312-77-5	0.97	0.28
119	undecane, 3-methyl-	1002-43-3	2.1	0.6
120	4-undecene, 4-methyl-	61142-40-3	0.86	0.18
121	decane, 2,3,6- trimethyl-	62238-12-4	0.71	0.18
122	cyclododecane	294-62-2	1.4	0.3
123	naphthalene, decahydro-2,6-dimethyl-	1618-22-0	1.4	0.3
124	naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.11	0.11
125	cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.53	0.11
126	5-heptenal, 2,6-dimethyl-	106-72-9	0.42	0.11
127	undecane, 2,4-dimethyl-	17312-80-0	0.16	0.15
128	undecane, 2,6-dimethyl-	17301-23-4	7.5	1.7
129	undecane, 2,7-dimethyl-	17301-24-5	0.40	0.37
130	undecane, 3,7-dimethyl-	17301-29-0	0.24	0.42
131	dimethyl-decahydronaphthalene		1.0	0.2
132	cyclopentane, 1-pentyl-2-propyl-	62199-51-3	0.26	0.05
133	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	3.0	0.6
134	1-octanol, 2-butyl-	3913-02-8	0.35	0.08
135	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.36	0.08
136	(E,E)(3S,8S),3,8-dimethyldeca-4,6-diene		0.47	0.10
137	cyclohexane, (4-methylpentyl)-	61142-20-9	2.7	0.5
138	dodecane, 6-methyl-	6044-71-9	0.80	0.15

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
139	dodecane, 5-methyl-	17453-93-9	0.57	0.12
140	dodecane, 4-methyl-	6117-97-1	1.8	0.4
141	undecane, 2,10-dimethyl-	17301-27-8	3.3	0.7
142	mixture		0.45	0.10
143	dodecane, 4,6-dimethyl-	61141-72-8	6.4	6.1
144	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.15	0.14
145	tridecane, 7-methyl-	26730-14-3	3.9	6.8
146	2(3H)-benzofuranone,3a,4,5,6-tetrahydro-3a,6,6-trimethyl-	16778-26-0	0.73	0.20
147	cyclohexane, 1,2-diethyl-1-methyl-	61141-79-5	0.24	0.25
148	6-tridecene, 7-methyl-	24949-42-6	2.3	0.7
149	5-tetradecene, (E)-	41446-66-6	0.63	0.17
150	tridecane, 5-methyl-	25117-31-1	0.32	0.31
151	undecane, 4,6-dimethyl-	17312-82-2	0.47	0.44
152	tetradecane	629-59-4	0.22	0.38
153	undecane, 6,6-dimethyl-	17312-76-4	0.30	0.51
154	dodecane, 2,5-dimethyl-	56292-65-0	2.5	0.7
155	cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.093	0.087
156	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-	54934-93-9	0.31	0.10
157	4-nonene, 2,3,3-trimethyl-, (E)-	63830-68-2	0.57	0.16
158	naphthalene, 2-butyldecahydro-	6305-52-8	0.32	0.09
159	tetradecane	629-59-4	1.0	0.3
160	octane, 2-cyclohexyl-	2883-05-8	2.6	0.8
161	tridecane, 4-methyl-	26730-12-1	1.5	0.4
162	tridecane, 2-methyl-	1560-96-9	2.0	0.6
163	undecane, 4,6-dimethyl-	17312-82-2	0.037	0.064
164	decane, 2,3,5,8-tetramethyl-		0.052	0.091
165	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-	54934-93-9	0.70	0.20
166	tridecane, 3-methyl-	6418-41-3	0.25	0.44

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
167	dodecane, 3-methyl-	17312-57-1	0.87	0.75
168	dodecane, 2,6,10-trimethyl-	3891-98-3	7.3	2.1
169	cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.027	0.047
170	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-	54823-94-8	0.25	0.07
171	tetradecane	629-59-4	7.3	2.0
172	tridecane, 4,8-dimethyl-	55030-62-1	1.5	1.4
173	tridecane, 3-ethyl-	13286-73-2	0.089	0.154
174	pentadecane	629-62-9	1.2	1.7
175	pentadecane	629-62-9	0.32	0.55
176	alkyl-cyclohexane		0.45	0.15
177	heptadecane, 7-methyl-	20959-33-5	0.17	0.29
178	c15-alkane		0.14	0.16
179	c15-alkane		0.16	0.15
180	decane, 1,1'-oxybis-	2456-28-2	0.65	0.63
181	1-octadecanol	112-92-5	0.45	0.78
182	dodecane, 2-methyl-8-propyl-	55045-07-3	2.9	0.8
183	pentadecane, 2-methyl-	1560-93-6	0.18	0.17
184	tetradecane, 3-methyl-	18435-22-8	0.13	0.22
185	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.091	0.080
186	7-hexadecene, (Z)-	35507-09-6	0.22	0.06
187	2-pentanone, 4-cyclohexyliden-3,3-diethyl-		0.11	0.10
188	pentadecane	629-62-9	1.6	0.5
189	dodecanoic acid	143-07-7	0.31	0.10
190	hexadecane	544-76-3	0.053	0.092
191	benzenamine, N-phenyl-	122-39-4	0.23	0.06
192	tetradecanoic acid	544-63-8	2.1	1.7
193	hexacosane	630-01-3	0.099	0.172
194	benzenesulfonamide, N-butyl-	3622-84-2	1.5	0.7

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
195	pentadecanoic acid	1002-84-2	0.36	0.14
196	1-hexadecanol	36653-82-4	0.097	0.174
197	1-hexadecene	629-73-2	0.049	0.085
198	alkane		0.53	0.92
199	alkane		2.2	3.6
200	9-hexadecenoic acid	2091-29-4	0.32	0.31
201	hexadecanoic acid	57-10-3	1.4	1.4
202	phthalate		0.081	0.140
203	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.44	0.31
204	ethanol, 2-(tetradecyloxy)-	2136-70-1	0.70	1.22
205	alkane		0.09	0.15
206	5-eicosane, (E)	74685-30-6	0.23	0.39
207	1-hexadecene	629-73-2	0.25	0.43
208	octadecane	593-45-3	0.025	0.043
Sum of tentatively identified compounds:			251.9	

1 CAS = Chemical Abstract Service

2 Average of 3, 55 ml TST samples, values listed are estimates.

Table 4-8
Tank BY-108 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)
136	(E,E)(3S,8S),3,8-dimethyldeca-4,6-diene		0.47	0.10
2	1-propene, 2-methyl-	115-11-7	2.1	0.4
3	1-propene, 2-methyl-	115-11-7	0.48	0.84
4	1-butene, 3-methyl-	563-45-1	0.51	0.88
1	1-propene, 2-methyl-	115-11-7	1.6	1.5
64	1-hexene, 4,5-dimethyl-	16106-59-5	0.11	0.20
45	1-octanol	111-87-5	0.12	0.20
100	1-undecene, 4-methyl-	74630-39-0	0.51	0.89
134	1-octanol, 2-butyl-	3913-02-8	0.35	0.08
207	1-hexadecene	629-73-2	0.25	0.43
37	1-octene	111-66-0	0.74	0.65
86	1-ethyl-2,2,6-trimethylcyclohexane		0.55	0.14
181	1-octadecanol	112-92-5	0.45	0.78
14	1-pentene, 4-methyl-	691-37-2	2.5	0.3
196	1-hexadecanol	36653-82-4	0.097	0.174
16	1-propene, 2-fluoro-	1184-60-7	0.47	0.82
197	1-hexadecene	629-73-2	0.049	0.085
18	1-pentene, 2-methyl-	763-29-1	2.6	1.6
19	1-hexene	592-41-6	3.0	2.6
34	1-heptene, 3-methyl-	4810-09-7	0.52	0.46
110	1-dodecene	112-41-4	0.38	0.08
43	1-octene	111-66-0	0.18	0.31
33	1-heptene, 6-methyl-	5026-76-6	0.25	0.43
24	1-pentene, 3,4-dimethyl-	7385-78-6	0.59	1.02
25	1-hexene, 5-methyl-	3524-73-0	0.53	0.91
50	1-nonene	124-11-8	0.31	0.27

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
23	1,3-pentadiene, 2-methyl-	1118-58-7	0.49	0.85
81	1,4-pentadiene, 2,3,4-trimethyl- & others		0.079	0.137
29	2-heptene	592-77-8	0.16	0.28
109	2-undecene, 8-methyl-	74630-44-7	0.38	0.12
97	2-nonanone and others	821-55-6	0.93	0.23
187	2-pentanone, 4-cyclohexyliden-3,3-diethyl-		0.11	0.10
66	2-heptanone, 6-methyl-	928-68-7	1.4	0.6
20	2-butanone	78-93-3	0.66	1.14
69	2-octanol	123-96-6	0.40	0.20
12	2-pentene, (Z)-	627-20-3	0.88	0.76
11	2-propanol	67-63-0	5.3	1.6
71	2-heptyl furan		0.22	0.23
146	2(3H)-benzofuranone,3a,4,5,6tetrahydro-3a,6,6-trimethyl-	16778-26-0	0.73	0.20
44	2H-pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.81	0.72
39	3-pentanol, 2-methyl- and others		0.11	0.19
58	3-heptanone	106-35-4	0.68	0.10
113	3-dodecene, (Z)-	7239-23-8	0.20	0.19
8	3-buten-1-ol	627-27-0	6.1	10.5
70	3-buten-2-ol	598-32-3	4.8	3.9
82	3-decyne	2384-85-2	0.51	0.17
62	3,4-nonadiene	37050-03-6	0.48	0.14
157	4-nonene, 2,3,3-trimethyl-, (E)-	63830-68-2	0.57	0.16
120	4-undecene, 4-methyl-	61142-40-3	0.86	0.18
65	4-nonyne	20184-91-2	0.13	0.23
149	5-tetradecene, (E)-	41446-66-6	0.63	0.17
99	5-undecene	4941-53-1	0.49	0.13
206	5-eicosane, (E)	74685-30-6	0.23	0.39
96	5-undecene	4941-53-1	1.0	0.3

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
126	5-heptenal, 2,6-dimethyl-	106-72-9	0.42	0.11
148	6-tridecene, 7-methyl-	24949-42-6	2.3	0.7
115	6-methylundecane	17302-33-9	3.4	0.9
186	7-hexadecene, (Z)-	35507-09-6	0.22	0.06
200	9-hexadecenoic acid	2091-29-4	0.32	0.31
198	alkane		0.53	0.92
199	alkane		2.2	3.6
205	alkane		0.09	0.15
176	alkyl-cyclohexane		0.45	0.15
191	benzenamine, N-phenyl-	122-39-4	0.23	0.06
52	benzene, ethyl and octane, 2-methyl-		0.54	0.05
53	benzene, 1,2-dimethyl-	95-47-6	0.40	0.69
54	benzene, 1,4-dimethyl-	106-42-3	0.35	0.61
59	benzene, 1,2-dimethyl-	95-47-6	0.38	0.06
194	benzenesulfonamide, N-butyl-	3622-84-2	1.5	0.7
103	bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-		0.41	0.09
5	butane, 2-methyl-	78-78-4	7.9	0.8
57	butane, 1,1'-oxybis-	142-96-1	0.17	0.15
178	c15-alkane		0.14	0.16
179	c15-alkane		0.16	0.15
95	c5-cyclohexane		0.69	0.14
13	cyclobutane, methyl-	598-61-8	0.92	0.80
122	cyclododecane	294-62-2	1.4	0.3
85	cyclohexaen, cyclopropyl-	32669-86-6	0.19	0.17
30	cyclohexane, methyl-	108-87-2	1.13	0.06
40	cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.11	0.20
48	cyclohexane, ethyl-	1678-91-7	0.46	0.11
49	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.82	0.19

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
61	cyclohexane, 1-ethyl-4-methyl-, trans-	6236-88-0	0.057	0.099
68	cyclohexane, 1,1,4,4-tetramethyl-		0.41	0.12
72	cyclohexane, 1-methyl-4-(1-methylethyl) & others		0.099	0.170
78	cyclohexane, 1,5-diethyl-2,3-dimethyl-	74663-66-4	0.52	0.25
83	cyclohexane, butyl-	1678-93-9	1.46	0.39
84	cyclohexane, 1-ethyl-4-methyl, cis-	4926-78-7	0.16	0.14
92	cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.47	0.12
98	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.28	0.26
125	cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.53	0.11
133	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	3.0	0.6
137	cyclohexane, (4-methylpentyl)-	61142-20-9	2.7	0.5
144	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.15	0.14
147	cyclohexane, 1,2-diethyl-1-methyl-	61141-79-5	0.24	0.25
156	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-	54934-93-9	0.31	0.10
165	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-	54934-93-9	0.70	0.20
169	cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.027	0.047
170	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-	54823-94-8	0.25	0.07
94	cyclohexane, 1-(cyclohexylmethyl)-4-methyl-	66826-95-7	0.80	0.19
75	cyclohexane, 1-methyl-4-(1-methylethyl)cis	6069-98-3	0.23	0.22
21	cyclopentane, methyl	96-37-7	2.1	0.3
27	cyclopentane, 1,2-dimethyl-, trans-	822-50-4	0.324	0.305
41	cyclopentane, 1,1,3-trimethyl-	4516-69-2	0.24	0.21
76	cyclopentane, 1-methyl-3-(2-methylpropyl)	29053-04-1	0.57	0.16
111	cyclopentane, (2-methylbutyl)-	53366-38-4	0.35	0.10
132	cyclopentane, 1-pentyl-2-propyl	62199-51-3	0.26	0.05
155	cyclopentane, 1-hexyl-3-methyl	61142-68-5	0.093	0.087
74	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.25	0.44
73	cyclopentanone, 2-methyl-4-(2-methylpropyl)	69770-96-3	0.16	0.27

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
7	cyclopropane, ethyl-	1191-96-4	7.3	0.8
28	cyclopropane, butyl-	930-57-4	2.5	0.3
77	cyclotetrasiloxane, octamethyl-	556-67-2	1.1	0.9
87	decane, 5-methyl-	13151-35-4	0.73	0.20
88	decane, 4-methyl-	2847-72-5	0.78	0.21
89	decane, 2-methyl-	6975-98-0	1.8	0.5
91	decane, 3-methyl-	13151-34-3	1.1	0.2
121	decane, 2,3,6- trimethyl-	62238-12-4	0.71	0.18
164	decane, 2,3,5,8-tetramethyl-		0.052	0.091
180	decane, 1,1'-oxybis-	2456-28-2	0.65	0.63
108	dimethyl-decahydronaphthalene		0.25	0.24
131	dimethyl-decahydronaphthalene		1.0	0.2
138	dodecane, 6-methyl-	6044-71-9	0.80	0.15
139	dodecane, 5-methyl-	17453-93-9	0.57	0.12
140	dodecane, 4-methyl-	6117-97-1	1.8	0.4
143	dodecane, 4,6-dimethyl-	61141-72-8	6.4	6.1
154	dodecane, 2,5-dimethyl-	56292-65-0	2.5	0.7
167	dodecane, 3-methyl-	17312-57-1	0.87	0.75
168	dodecane, 2,6,10-trimethyl-	3891-98-3	7.3	2.1
182	dodecane, 2-methyl-8-propyl-	55045-07-3	2.9	0.8
189	dodecanoic acid	143-07-7	0.31	0.10
204	ethanol, 2-(tetradecyloxy)-	2136-70-1	0.70	1.22
93	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.37	0.10
9	furan	110-00-9	0.55	0.96
22	furan, tetrahydro-	109-99-9	8.5	2.0
177	heptadecane, 7-methyl-	20959-33-5	0.17	0.29
35	heptane, 2,3,5-trimethyl-	20278-85-7	0.65	1.12
36	heptane, 2,3,6-trimethyl-	4032-93-3	1.26	1.10

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
38	heptane, 3-methyl-	589-81-1	0.19	0.32
47	heptane, 2,6-dimethyl-	1072-05-5	0.56	0.07
51	heptane, 2,3-dimethyl-	3074-71-3	0.09	0.16
55	heptane, 3,5-dimethyl-	926-82-9	0.073	0.126
63	heptane, 4-(1-methylethyl)-	52896-87-4	0.15	0.26
193	hexacosane	630-01-3	0.099	0.172
185	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.091	0.080
190	hexadecane	544-76-3	0.053	0.092
201	hexadecanoic acid	57-10-3	1.4	1.4
203	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.44	0.31
46	hexamethylcyclotrisiloxane	541-05-9	0.13	0.22
42	hexanal, 3-methyl-	19269-28-4	0.24	0.42
26	hexane, 2-methyl-	591-76-4	1.34	0.05
6	methane, trichlorofluoro-	75-69-4	11.9	13.0
31	mixture		0.14	0.24
60	mixture		0.069	0.119
142	mixture		0.45	0.10
90	naphthalene, decahydro-, trans-	493-02-7	1.1	0.3
105	naphthalene, decahydro-2-methyl-	2958-76-1	2.2	0.6
112	naphthalene, decahydro-2-methyl-	2958-76-1	5.9	1.6
114	naphthalene, decahydro-2-methyl-	2958-76-1	0.21	0.19
123	naphthalene, decahydro-2,6-dimethyl-	1618-22-0	1.4	0.3
124	naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.11	0.11
135	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.36	0.08
158	naphthalene, 2-butyldecahydro-	6305-52-8	0.32	0.09
67	nonane, 4-methyl-	17301-94-9	0.57	0.25
79	nonane, 2,6-dimethyl-	17302-28-2	2.2	1.1
101	nonane, 3,7-dimethyl-	17302-32-8	0.80	1.39

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
208	octadecane	593-45-3	0.025	0.043
56	octane, 3-methyl and c2-benzene		0.43	0.74
80	octane, 6-ethyl-2-methyl-	62016-19-7	0.19	0.20
160	octane, 2-cyclohexyl-	2883-05-8	2.6	0.8
10	oxirane, ethenyl-	930-22-3	0.8	1.4
174	pentadecane	629-62-9	1.2	1.7
175	pentadecane	629-62-9	0.32	0.55
183	pentadecane, 2-methyl-	1560-93-6	0.18	0.17
188	pentadecane	629-62-9	1.6	0.5
195	pentadecanoic acid	1002-84-2	0.36	0.14
15	pentane, 2-methyl-	107-83-5	15.1	0.9
17	pentane, 3-methyl-	96-14-0	2.5	0.2
202	phthalate		0.081	0.140
32	propane, 2-nitro- & others		0.14	0.23
152	tetradecane	629-59-4	0.22	0.38
159	tetradecane	629-59-4	1.0	0.3
171	tetradecane	629-59-4	7.3	2.0
184	tetradecane, 3-methyl-	18435-22-8	0.13	0.22
192	tetradecanoic acid	544-63-8	2.1	1.7
145	tridecane, 7-methyl-	26730-14-3	3.9	6.8
150	tridecane, 5-methyl-	25117-31-1	0.32	0.31
161	tridecane, 4-methyl-	26730-12-1	1.5	0.4
162	tridecane, 2-methyl-	1560-96-9	2.0	0.6
166	tridecane, 3-methyl-	6418-41-3	0.25	0.44
172	tridecane, 4,8-dimethyl-	55030-62-1	1.5	1.4
173	tridecane, 3-ethyl-	13286-73-2	0.089	0.154
102	undecane, 5-methyl-	1632-70-8	2.9	0.8
104	undecane, 4-methyl-	2980-69-0	0.36	0.09

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
106	undecane, 3,8-dimethyl-	17301-30-3	1.0	0.9
107	undecane, 4,7-dimethyl-	17301-32-5	0.77	1.34
116	undecane, 4-methyl-	2980-69-0	1.9	0.5
117	undecane, 2-methyl-	7045-71-8	3.8	1.0
118	undecane, 2,3-dimethyl-	17312-77-5	0.97	0.28
119	undecane, 3-methyl-	1002-43-3	2.1	0.6
127	undecane, 2,4-dimethyl-	17312-80-0	0.16	0.15
128	undecane, 2,6-dimethyl-	17301-23-4	7.5	1.7
129	undecane, 2,7-dimethyl-	17301-24-5	0.40	0.37
130	undecane, 3,7-dimethyl-	17301-29-0	0.24	0.42
141	undecane, 2,10-dimethyl-	17301-27-8	3.3	0.7
151	undecane, 4,6-dimethyl-	17312-82-2	0.47	0.44
153	undecane, 6,6-dimethyl-	17312-76-4	0.30	0.51
163	undecane, 4,6-dimethyl-	17312-82-2	0.037	0.064
Sum of tentatively identified compounds:			251.9	

1 CAS = Chemical Abstract Service.

2 Average of 3, 55 ml TST samples, values listed are estimates.

Table 4-9
Tank BY-108 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)
15	pentane, 2-methyl-	107-83-5	15.1	0.9
6	methane, trichlorofluoro-	75-69-4	11.9	13.0
22	furan, tetrahydro-	109-99-9	8.5	2.0
5	butane, 2-methyl-	78-78-4	7.9	0.8
128	undecane, 2,6-dimethyl-	17301-23-4	7.5	1.7
168	dodecane, 2,6,10-trimethyl-	3891-98-3	7.3	2.1
7	cyclopropane, ethyl-	1191-96-4	7.3	0.8
171	tetradecane	629-59-4	7.3	2.0
143	dodecane, 4,6-dimethyl-	61141-72-8	6.4	6.1
8	3-buten-1-ol	627-27-0	6.1	10.5
112	naphthalene, decahydro-2-methyl-	2958-76-1	5.9	1.6
11	2-propanol	67-63-0	5.3	1.6
70	3-buten-2-ol	598-32-3	4.8	3.9
145	tridecane, 7-methyl-	26730-14-3	3.9	6.8
117	undecane, 2-methyl-	7045-71-8	3.8	1.0
115	6-methylundecane	17302-33-9	3.4	0.9
141	undecane, 2,10-dimethyl-	17301-27-8	3.3	0.7
19	1-hexene	592-41-6	3.0	2.6
182	dodecane, 2-methyl-8-propyl-	55045-07-3	2.9	0.8
102	undecane, 5-methyl-	1632-70-8	2.9	0.8
137	cyclohexane, (4-methylpentyl)-	61142-20-9	2.7	0.5
18	1-pentene, 2-methyl-	763-29-1	2.6	1.6
160	octane, 2-cyclohexyl-	2883-05-8	2.6	0.8
17	pentane, 3-methyl-	96-14-0	2.5	0.2
154	dodecane, 2,5-dimethyl-	56292-65-0	2.5	0.7
14	1-pentene, 4-methyl-	691-37-2	2.5	0.3

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	cyclopropane, butyl-	930-57-4	2.5	0.3
148	6-tridecene, 7-methyl-	24949-42-6	2.3	0.7
79	nonane, 2,6-dimethyl-	17302-28-2	2.2	1.1
199	alkane		2.2	3.6
105	naphthalene, decahydro-2-methyl-	2958-76-1	2.2	0.6
192	tetradecanoic acid	544-63-8	2.1	1.7
119	undecane, 3-methyl-	1002-43-3	2.1	0.6
21	cyclopentane, methyl-	96-37-7	2.1	0.3
2	1-propene, 2-methyl-	115-11-7	2.1	0.4
162	tridecane, 2-methyl-	1560-96-9	2.0	0.6
116	undecane, 4-methyl-	2980-69-0	1.9	0.5
89	decane, 2-methyl-	6975-98-0	1.8	0.5
140	dodecane, 4-methyl-	6117-97-1	1.8	0.4
1	1-propene, 2-methyl-	115-11-7	1.6	1.5
188	pentadecane	629-62-9	1.6	0.5
161	tridecane, 4-methyl-	26730-12-1	1.5	0.4
172	tridecane, 4,8-dimethyl-	55030-62-1	1.5	1.4
194	benzenesulfonamide, N-butyl-	3622-84-2	1.5	0.7
83	cyclohexane, butyl-	1678-93-9	1.46	0.39
122	cyclododecane	294-62-2	1.4	0.3
66	2-heptanone, 6-methyl-	928-68-7	1.4	0.6
201	hexadecanoic acid	57-10-3	1.4	1.4
123	naphthalene, decahydro-2,6-dimethyl-	1618-22-0	1.4	0.3
26	hexane, 2-methyl-	591-76-4	1.34	0.05
36	heptane, 2,3,6-trimethyl-	4032-93-3	1.26	1.10
174	pentadecane	629-62-9	1.2	1.7
30	cyclohexane, methyl-	108-87-2	1.13	0.06
77	cyclotetrasiloxane, octamethyl-	556-67-2	1.1	0.9

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
90	naphthalene, decahydro-, trans-	493-02-7	1.1	0.3
91	decane, 3-methyl-	13151-34-3	1.1	0.2
131	dimethyl-decahydronaphthalene		1.0	0.2
106	undecane, 3,8-dimethyl-	17301-30-3	1.0	0.9
96	5-undecene	4941-53-1	1.0	0.3
159	tetradecane	629-59-4	1.0	0.3
118	undecane, 2,3-dimethyl-	17312-77-5	0.97	0.28
97	2-nonanone and others		0.93	0.23
13	cyclobutane, methyl-	598-61-8	0.92	0.80
12	2-pentene, (Z)-	627-20-3	0.88	0.76
167	dodecane, 3-methyl-	17312-57-1	0.87	0.75
120	4-undecene, 4-methyl-	61142-40-3	0.86	0.18
49	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.82	0.19
44	2H-pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.81	0.72
101	nonane, 3,7-dimethyl-	17302-32-8	0.80	1.39
10	oxirane, ethenyl-	930-22-3	0.8	1.4
138	dodecane, 6-methyl-	6044-71-9	0.80	0.15
88	decane, 4-methyl-	2847-72-5	0.78	0.21
107	undecane, 4,7-dimethyl-	17301-32-5	0.77	1.34
56	octane, 3-methyl and c2-benzene		0.43	0.74
37	1-octene	111-66-0	0.74	0.65
146	2(3H)-benzofuranone,3a,4,5,6tetrahydro-3a,6,6-trimethyl-	16778-26-0	0.73	0.20
87	decane, 5-methyl-	13151-35-4	0.73	0.20
121	decane, 2,3,6- trimethyl-	62238-12-4	0.71	0.18
204	ethanol, 2-(tetradecyloxy)-	2136-70-1	0.70	1.22
95	c5-cyclohexane		0.69	0.14
58	3-heptanone	106-35-4	0.68	0.10
20	2-butanone	78-93-3	0.66	1.14

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
35	heptane, 2,3,5-trimethyl-	20278-85-7	0.65	1.12
180	decane, 1,1'-oxybis-	2456-28-2	0.65	0.63
149	5-tetradecene, (E)-	41446-66-6	0.63	0.17
133	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	3.0	0.6
24	1-pentene, 3,4-dimethyl-	7385-78-6	0.59	1.02
67	nonane, 4-methyl-	17301-94-9	0.57	0.25
76	cyclopentane, 1-methyl-3-(2-methylpropyl)	29053-04-1	0.57	0.16
139	dodecane, 5-methyl-	17453-93-9	0.57	0.12
157	4-nonene, 2,3,3-trimethyl-, (E)-	63830-68-2	0.57	0.16
47	heptane, 2,6-dimethyl-	1072-05-5	0.56	0.07
9	furan	110-00-9	0.55	0.96
125	cyclohexane, 1-methyl-2-pentyl-	54411-01-7	0.53	0.11
25	1-hexene, 5-methyl-	3524-73-0	0.53	0.91
198	alkane		0.53	0.92
34	1-heptene, 3-methyl-	4810-09-7	0.52	0.46
78	cyclohexane, 1,5-diethyl-2,3-dimethyl-	74663-66-4	0.52	0.25
4	1-butene, 3-methyl-	563-45-1	0.51	0.88
100	1-undecene, 4-methyl-	74630-39-0	0.51	0.89
82	3-decyne	2384-85-2	0.51	0.17
99	5-undecene	4941-53-1	0.49	0.13
23	1,3-pentadiene, 2-methyl-	1118-58-7	0.49	0.85
62	3,4-nonadiene	37050-03-6	0.48	0.14
3	1-propene, 2-methyl-	115-11-7	0.48	0.84
151	undecane, 4,6-dimethyl-	17312-82-2	0.47	0.44
16	1-propene, 2-fluoro-	1184-60-7	0.47	0.82
48	cyclohexane, ethyl-	1678-91-7	0.46	0.11
176	alkyl-cyclohexane		0.45	0.15
181	1-octadecanol	112-92-5	0.45	0.78

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
142	mixture		0.45	0.10
203	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.44	0.31
126	5-heptenal, 2,6-dimethyl-	106-72-9	0.42	0.11
53	benzene, 1,2-dimethyl-	95-47-6	0.40	0.69
69	2-octanol	123-96-6	0.40	0.20
129	undecane, 2,7-dimethyl-	17301-24-5	0.40	0.37
109	2-undecene, 8-methyl-	74630-44-7	0.38	0.12
59	benzene, 1,2-dimethyl-	95-47-6	0.38	0.06
110	1-dodecene	112-41-4	0.38	0.08
135	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.36	0.08
195	pentadecanoic acid	1002-84-2	0.36	0.14
104	undecane, 4-methyl-	2980-69-0	0.36	0.09
54	benzene, 1,4-dimethyl-	106-42-3	0.35	0.61
111	cyclopentane, (2-methylbutyl)-	53366-38-4	0.35	0.10
134	1-octanol, 2-butyl-	3913-02-8	0.35	0.08
27	cyclopentane, 1,2-dimethyl-, trans-	822-50-4	0.324	0.305
150	tridecane, 5-methyl-	25117-31-1	0.32	0.31
200	9-hexadecenoic acid	2091-29-4	0.32	0.31
158	naphthalene, 2-butyldecahydro-	6305-52-8	0.32	0.09
175	pentadecane	629-62-9	0.32	0.55
50	1-nonene	124-11-8	0.31	0.27
189	dodecanoic acid	143-07-7	0.31	0.10
156	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-	54934-93-9	0.31	0.10
153	undecane, 6,6-dimethyl-	17312-76-4	0.30	0.51
98	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.28	0.26
132	cyclopentane, 1-pentyl-2-propyl-	62199-51-3	0.26	0.05
74	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.25	0.44
108	dimethyl-decahydronaphthalene		0.25	0.24

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
170	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-	54823-94-8	0.25	0.07
33	1-heptene, 6-methyl-	5026-76-6	0.25	0.43
207	1-hexadecene	629-73-2	0.25	0.43
166	tridecane, 3-methyl-	6418-41-3	0.25	0.44
130	undecane, 3,7-dimethyl-	17301-29-0	0.24	0.42
42	hexanal, 3-methyl-	19269-28-4	0.24	0.42
41	cyclopentane, 1,1,3-trimethyl-	4516-69-2	0.24	0.21
147	cyclohexane, 1,2-diethyl-1-methyl-	61141-79-5	0.24	0.25
191	benzenamine, N-phenyl-	122-39-4	0.23	0.06
75	cyclohexane, 1-methyl-4-(1-methylethyl)cis	6069-98-3	0.23	0.22
206	5-eicosane, (E)	74685-30-6	0.23	0.39
71	2-heptyl furan		0.22	0.23
186	7-hexadecene, (Z)-	35507-09-6	0.22	0.06
152	tetradecane	629-59-4	0.22	0.38
114	naphthalene, decahydro-2-methyl-	2958-76-1	0.21	0.19
113	3-dodecene, (Z)-	7239-23-8	0.20	0.19
165	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl-	54934-93-9	0.70	0.20
80	octane, 6-ethyl-2-methyl-	62016-19-7	0.19	0.20
38	heptane, 3-methyl-	589-81-1	0.19	0.32
85	cyclohexane, cyclopropyl-	32669-86-6	0.19	0.17
94	cyclohexane, 1-(cyclohexylmethyl)-4-methyl-	66826-95-7	0.80	0.19
183	pentadecane, 2-methyl-	1560-93-6	0.18	0.17
43	1-octene	111-66-0	0.18	0.31
57	butane, 1,1'-oxybis-	142-96-1	0.17	0.15
177	heptadecane, 7-methyl-	20959-33-5	0.17	0.29
72	cyclohexane, 1-methyl-4-(1-methylethyl) & others		0.099	0.170
179	c15-alkane		0.16	0.15
73	cyclopentanone, 2-methyl-4-(2-methylpropyl)	69770-96-3	0.16	0.27

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
127	undecane, 2,4-dimethyl-	17312-80-0	0.16	0.15
84	cyclohexane, 1-ethyl-4-methyl, cis	4926-78-7	0.16	0.14
29	2-heptene	592-77-8	0.16	0.28
144	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.15	0.14
63	heptane, 4-(1-methylethyl)-	52896-87-4	0.15	0.26
31	mixture		0.14*	0.24
178	c15-alkane		0.14	0.16
32	propane, 2-nitro- & others		0.14	0.23
86	1-ethyl-2,2,6-trimethylcyclohexane		0.55	0.14
81	1,4-pentadiene, 2,3,4-trimethyl- & others		0.079	0.137
184	tetradecane, 3-methyl-	18435-22-8	0.13	0.22
65	4-nonyne	20184-91-2	0.13	0.23
46	hexamethylcyclotrisiloxane	541-05-9	0.13	0.22
92	cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.47	0.12
45	1-octanol	111-87-5	0.12	0.20
68	cyclohexane, 1,1,4,4-tetramethyl-		0.41	0.12
40	cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.11	0.20
124	naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.11	0.11
39	3-pentanol, 2-methyl and others		0.11	0.19
64	1-hexene, 4,5-dimethyl-	16106-59-5	0.11	0.20
187	2-pentanone, 4-cyclohexayliden-3,3-diethyl-		0.11	0.10
93	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.37	0.10
136	(E,E)(3S,8S),3,8-dimethyldeca-4,6-diene		0.47	0.10
193	hexacosane	630-01-3	0.099	0.172
196	1-hexadecanol	36653-82-4	0.097	0.174
155	cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.093	0.087
185	hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.091	0.080
51	heptane, 2,3-dimethyl-	3074-71-3	0.09	0.16

WHC-SD-WM-ER-422 REV. 2

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
103	bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-		0.41	0.09
205	alkane		0.09	0.15
173	tridecane, 3-ethyl-	13286-73-2	0.089	0.154
202	phthalate		0.081	0.140
55	heptane, 3,5-dimethyl-	926-82-9	0.073	0.126
60	mixture		0.069	0.119
61	cyclohexane, 1-ethyl-4-methyl-, trans-	6236-88-0	0.057	0.099
190	hexadecane	544-76-3	0.053	0.092
164	decane, 2,3,5,8-tetramethyl-		0.052	0.091
52	benzene, ethyl and octane, 2-methyl-		0.54	0.05
197	1-hexadecene	629-73-2	0.049	0.085
163	undecane, 4,6-dimethyl-	17312-82-2	0.037	0.064
169	cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.027	0.047
208	octadecane	593-45-3	0.025	0.043
Sum of tentatively identified compounds:			251.9	

1 CAS = Chemical Abstract Service.

2 Average of 3, 55 ml TST samples, values listed are estimates.