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Title/Desc:

TANK 241TY103 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
8/1994 & 4/1995

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

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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-TY-103 Headspace Gas and Vapor Characterization Results for Samples Collected in August 1994 and April 1995

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Acronyms and Abbreviations

CES	consensus exposure standard
EPA	Environmental Protection Agency
GC	gas chromatograph
GC/MS	gas chromatograph/mass spectrometer
ISS	in situ sampling
LFL	lower flammability limit
MS	mass spectrometer
NFPA	National Fire Protection Association
NPH	normal paraffinic hydrocarbon
ORNL	Oak Ridge National Laboratory
PNL	Pacific Northwest Laboratory
ppmv	parts per million by volume, 1 ppmv = 10 ⁻⁴ vol%
TST	triple sorbent trap
vol%	percent by volume, 1 vol% = 10,000 ppmv
VSS	vapor sampling system
WHC	Westinghouse Hanford Company

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Tank 241-TY-103 Headspace Gas and Vapor Characterization Results
for Samples Collected in August 1994 and April 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank TY-103 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 April 1995 sampling event, but also includes selected results of the August 1994 sampling event. The tank TY-103 headspace was sampled in August 1994 in accordance with *Safety Assessment for Gas Sampling All Ferrocyanide Tanks* (Farley 1991), and in April 1995 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 was collected to help in the evaluation of 1) headspace flammability, and 2) identification and quantification of compounds of toxicological concern.

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). However, current governing operating specifications for Watchlist tanks, such as tank TY-103, 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 TY-103 was vapor sampled in August 1994 using the *in situ* sampling (ISS) method, and again in April 1995 using the more robust vapor sampling system (VSS) method. Because the ISS sample volume flow measurement used during the August 1994 event was inherently less accurate than that of the VSS, the sorbent trap samples from the ISS event are not generally considered to be equivalent to those from the VSS sampling event (Huckaby and Babad 1995). Furthermore, there are other discrepancies between results from the ISS and VSS methods that are not completely 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 August 1994 ISS event are presented below, because this analyte was not sampled for during the VSS event. Huckaby and Babad (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 April 1995 VSS sampling event.

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

1.4 Tank Headspace Dynamics

Tank TY-103 is the third tank in a 3-tank cascade with tanks TY-101 and TY-102. It is connected to tank TY-102 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade line. Tanks TY-101 and TY-102 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 TY-102 or tank TY-102 may be transferred to tank TY-103 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for TY-102 to assess the potential effect on tank TY-103.

The cascade of tanks TY-101, TY-102, and TY-103 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 August 1994 *In Situ* Sampling Event

Tank TY-103 was sampled using ISS methods on August 5, 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 7.9 m below the top of the flange on riser 3, between 9:45 a.m. and 10:45 a.m.

Huckaby and Babad (1995) give a general description of the ISS method and equipment. Pingel (1994) provides field sampling information for the tank TY-103 August 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.

2.2 April 1995 Vapor Sampling System Sampling Event

Headspace gas and vapor samples were collected from tank TY-103 using the VSS on April 11, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-TY-103 Tank Characterization Plan* (Homi 1995). The tank headspace temperature was determined to be 15.9 °C. Air from the tank TY-103 headspace was withdrawn from a single elevation via a 5.5-m long heated sampling probe mounted in riser 8, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 40 °C. All tank air samples were collected between 10:37 a.m. and 2:09 p.m., with no sampling anomalies noted.

Sampling media for the VSS event 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 14 field blanks provided by the laboratories.

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

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor given in Table 3-1 has been adjusted to tank conditions as given in Section 3.3. Inorganic analyte sorbent traps and SUMMATM canister samples were prepared and analyzed by PNL (Ligotke et al. 1995).

Analyses of the VSS event inorganic vapor sorbent traps were performed within 9 days of sample collection, analyses of VSS event SUMMATM canisters for inorganic compounds were performed 7 days after sample collection, and analyses of the ISS event hydrogen cyanide sorbent traps were performed 35 days after sample collection (Ligotke 1995). This satisfied the 60-day holding time requirement of the WHC quality assurance project plan (Keller 1994). Though no holding time study has been performed to address the stability of compounds in SUMMATM canisters in the chemical matrix of the tank samples, these inorganic compounds (i.e., the permanent gases) would be expected to be very stable in the SUMMATM canisters, and the results may not have been affected even if the 60 day holding time requirements had been exceeded. All sample preparation and analyses were performed at PNL quality assurance impact level 2, except for the hydrogen cyanide results, which were produced at PNL quality assurance impact level 3.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The concentration of ammonia in the headspace of TY-103 was measured to be 49 ppmv. Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 1040 ppmv in BY-108 (McVeety et al. 1995). Given the LFL of ammonia in air is about 15 % by volume (vol%), the measured 49 ppmv corresponds to less than 0.04 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank TY-103 was determined to be < 93 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, a 93 ppmv hydrogen concentration in tank TY-103 would correspond to about 0.23 % of its LFL. At this level, hydrogen is not a flammability concern in tank TY-103.

The reported nitrous oxide concentration in tank TY-103, 159 ppmv, is typical of other waste tanks sampled to date. Nitrous oxide has been measured in other passively ventilated waste tanks at average concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as 878 ppmv in tank U-103 (Ligotke et al. 1995b). 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 TY-103 headspace.

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

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank TY-103 headspace was measured as < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide has not been measured at very high levels in any of the waste tanks. The highest level measured to date was [26.7 ppmv] in tank C-103² (Huckaby and Story 1994).

The carbon dioxide concentration in the tank TY-103 headspace, measured at an average 121 ppmv, is significantly lower than it is in ambient air. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient in the waste tank headspaces. The 2 ambient air samples collected at the start of the tank TY-103 April 1995 sampling event, for example, were measured to have an average 356 ppmv of carbon dioxide. The 121 ppmv of carbon dioxide in the tank TY-103 headspace is typical of values for the waste tanks sampled to-date.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank TY-103 headspace were determined to be 0.10 ppmv and ≤ 0.02 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank TY-103. The measurable presence of nitric oxide is not uncommon in the waste tank headspaces, and may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank TY-103 headspace.

The water vapor concentration of tank TY-103 was determined to be about 11.6 mg/L, at the measured tank headspace temperature of 15.9 °C and pressure of 994.3 mbar (745.9 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 15.4 mbar (11.6 torr), to a dew point of 13.5 °C, and to a relative humidity of 85 %.

Silica gel sorbent traps were used to sample for tritium. It is assumed that tritium produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Radiochemical analysis of the silica gel trap indicated the total activity of the headspace to be less than 50 pCi/L (WHC 1995b).

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.

3.4 Hydrogen Cyanide

Analysis of the hydrogen cyanide specific sorbent traps indicated the concentration of this analyte to be below 0.01 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 TY-103. 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 TY-103 headspace are nitrous oxide and ammonia. These have been detected in most tank headspaces sampled to date and, along with hydrogen, are usually the most abundant species. The concentrations of ammonia and nitrous oxide are typical of other waste tanks that have been sampled.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are satisfactory for the methods used. Relative standard deviations range from 1.1 % for water vapor to about 23 % for nitrous oxide results. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank TY-103 headspace were sampled using SUMMA™ canisters, which were prepared and analyzed by PNL, and triple sorbent traps (TSTs), which were prepared and analyzed by ORNL. PNL and ORNL both used a gas chromatograph (GC) and 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. (1995a) and Ligothke et al. (1995a).

SUMMA™ sample results produced by PNL should be considered to be the primary organic vapor data for tank TY-103. These results were produced at PNL quality assurance impact level 2, and all PNL analyses were completed 9 days after sample collection, well below the specified 60-day holding time (Keller 1994).

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

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

4.1 Positively Identified Organic Compounds

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained 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 39 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of vapor data on tank C-103.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMA™ samples. All compounds in Table 4-1 were analyzed according to the TO-14 methodology, except for methane, which was analyzed with the inorganic gases (Ligothke et al. 1995a). Only 6 of the 39 TO-14 target analytes (trichlorofluoromethane, 1,1,2-trichloro-1,2,2-trifluoroethane, trichloromethane, tetrachloromethane, toluene, and tetrachloromethane) and only 10 of the 14 additional target analytes were measured to be above the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMA™ canister samples.

Jenkins et al. (1995a) report the positive identification of 24 of 27 target analytes in TST samples. Dichloromethane, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected. Despite calibration of the instrument over about a 20-fold concentration range, none of the positively identified compounds were within the calibration range of the instrument in all 4 TST samples. The average concentrations of the positively identified analytes, from the analysis of 4 TSTs, are given in Tables 4-2 and 4-3. Table 4-2 lists those compounds for which their practical holding time was not exceeded, and Table 4-3 lists the positively identified analytes which did exceed their practical holding times. Tables 4-2 and 4-3 are mutually exclusive, so that no compound appears in both tables.

The ORNL practical holding time is defined as the holding time for which there is a 15 % risk that the concentration of an analyte in the sample will be below its initial concentration. As indicated in Table 4-4, butanal and 1-butanol exceeded their practical holding times, and may have been affected by the 25 day period between sample collection and analysis (Jenkins 1995b). Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the practical holding times of butanal, and 1-butanol are 1 and 17 days, respectively. It is worth noting that the contractual holding time for the TST samples was 60 days.

Both PNL and ORNL report target analyte concentrations in ppmv of analyte in dry air. To correct for the measured water vapor content of tank TY-103 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.985.

Eleven target analytes were common to both TST and SUMMA™ analyses. Table 4-4 lists these, and their reported average concentrations in TST and SUMMA™ samples. Results from these 2 sampling and analytical methods are in fairly good agreement. As indicated in Table 4-4, the reported concentrations of propanone and n-hexane were significantly higher in SUMMA™ samples than in TST samples. The target analytes are generally only present at very low concentrations, however, and none are near levels of concern.

n-Tridecane is the only analyte in Tables 4-1 through 4-3 to be measured above 1 ppmv. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

4.2 Tentatively Identified Organic Compounds

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

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and 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 tentatively identified compounds recovered from SUMMA™ samples, in the order by which the eluted chromatographically, are given in Table 4-5 with estimated concentrations. Only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-6 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table 4-6 are all 4-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Because the list of tentatively identified organic compounds in TST samples is rather long and locating any given compound may be difficult, the list has been sorted both alphanumerically by compound name in Table 4-7, and also in order of decreasing estimated concentrations in Table 4-8. Numbers in the first columns of Tables 4-7 and 4-8 (Cmpd #) identify the location of the compound in Table 4-6. Estimated concentrations in Tables 4-5 through 4-8 are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Ligotke et al. (1995a), respectively, and should be reviewed before this data is used for decision making. Concentrations given in Tables 4-5 through 4-8 should be considered rough estimates.

4.3 Discussion of Organic Compounds

The organic compounds listed in Tables 4-1 through 4-8 may be classified as either 1) organic compounds added to tank TY-103 as waste that are still evaporating, or 2) organic compounds that have been generated by reactions of the original waste.

Organic compounds in the first category, those that were placed into the tank as waste, include the semivolatile straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction processes. These alkanes (i.e., n-undecane, n-dodecane, n-tridecane, n-tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). About 90 % of the total estimated organic vapor in tank TY-103 TST samples is due to n-dodecane, n-tridecane, and n-tetradecane. The same 3 compounds account for about 82 % of the total estimated organic vapor concentration in SUMMA™ samples.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 9 and 11 in Table 4-6) may also have been sent to tank TY-103 with other wastes. Small quantities of siloxanes may have been introduced to the waste tank through their use as defoaming agents, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser. These have also been observed in TST blanks, however, and they may be present as artifacts of the gas chromatography process.

The absence of tributyl phosphate in the tank TY-103 samples does not necessarily indicate it is not present in the headspace or the waste. The relatively high concentrations of the tributyl phosphate diluents (i.e., n-dodecane, n-tridecane, and n-tetradecane) and their degradation products is reason to expect tributyl phosphate may be present in the tank waste. 1-Butanol, which is one of the most abundant organic compounds identified in tank TY-103 TST samples, is known to be a product of the hydrolysis of tributyl phosphate. Furthermore, informal tests by ORNL indicate that tributyl phosphate is adsorbed by the glass fiber filters used during sampling to protect the samples from radiolytic particulate contamination. Based on these considerations, the lack of tributyl phosphate in the tank TY-103 headspace samples should not be taken as proof it is not present in the headspace or the waste.

A relatively large number of halogenated organic compounds were detected in samples from tank TY-103, including trichlorofluoromethane (which is frequently detected in the waste tanks), trichloromethane, tetrachloromethane, 1,1,2-trichloro-1,2,2-trifluoroethane, and tetrachloroethene. These compounds are frequently used as cleaning solvents and may have been sent to the waste tanks when they became radiologically contaminated. Trichlorofluoromethane may be associated with the foam used to seal concrete pit covers on tank TY-103.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-6 fall into this category, including the alcohols, aldehydes, alkenes, ketones, nitriles, and volatile alkanes, all of which have been associated with the degradation of the NPHs.

The total organic vapor concentration of tank TY-103 was estimated by Jenkins et al. (1995a) to be about 60 mg/m³ from the analysis of 4 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMA™ samples from tank TY-103 provides an estimated total organic vapor concentration of 31.8 mg/m³. Compared to other waste tanks that have been sampled, tank TY-103 has a relatively high concentration of organic vapors.

In summary, the organic vapors in tank TY-103 clearly indicate the presence of the semivolatile NPHs and their degradation products in the tank waste. Tributyl phosphate was not detected in any of the headspace samples, but there is strong evidence that it is also present in the waste.

5.0 SUMMARY

The tank TY-103 headspace was sampled in August 1994 and April 1995 for gases and vapors to address flammability and industrial hygiene concerns. Results unique to the August 1994 event and essentially all results from the April 1995 event have been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank TY-103 Gas and Vapor Sample Type and Number for April 1995 Sampling Event

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.2	Organic vapors	4 tank air samples
		1.0	Organic vapors	4 tank air samples
		4.0	Organic vapors	4 tank air samples
				+ 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blank + 3 field blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank + 3 field blanks
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blank + 3 field blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks + 3 field blanks
	SUMMA™ canister	6.0	Carbon Dioxide, Carbon Monoxide, Hydrogen, Methane, Nitrous Oxide, Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
 Tank TY-103 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	49	1	2
Carbon Dioxide, CO ₂	124-38-9	SUMMA TM	3	121	7	6
Carbon Monoxide, CO	630-08-0	SUMMA TM	3	< 12	--	--
Hydrogen, H ₂	1333-74-0	SUMMA TM	3	< 93	--	--
Hydrogen Cyanide ³ , HCN	74-90-8	Sorbent Trap	3	< 0.01	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.10	0.02	20
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.06	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA TM	3	159	37	23
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	15,500 (11.6 mg/L)	200 (0.1 mg/L)	1.1

¹ CAS = Chemical Abstracts Service.

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

³ Results for hydrogen cyanide are from the August 1994 ISS event.

Table 4-1
Tank TY-103 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	Ethanenitrile (acetonitrile)	75-05-8	0.075	0.003	4
2	Propanone (acetone)	67-64-1	0.13	0.01	7
3	Trichlorofluoromethane	75-69-4	0.14	0.01	8
4	1,1,2-trichloro-1,2,2-trifluoroethane	76-13-1	0.007	0.001	8
5	Propanenitrile	107-12-0	0.017	0.006	36
6	1-Propanol	71-23-8	0.023	0.007	30
7	2-Butanone	78-93-3	0.017	0.007	39
8	n-Hexane	110-54-3	0.38	0.02	4
9	Trichloromethane (chloroform)	67-66-3	0.008	0.0002	2
10	Tetrahydrofuran	109-99-9	0.022	0.001	4
11	Tetrachloromethane (carbon tetrachloride)	56-23-5	0.029	0.002	6
12	n-Heptane	142-82-5	0.006	0.0004	7
13	Pyridine	110-86-1	0.012	0.008	67
14	Toluene	108-88-3	0.013	0.001	5
15	Tetrachloroethene	127-18-4	0.010	0.0004	4
16	n-Decane	124-18-5	0.006	< 0.01	--
17	Methane	74-82-8	< 12	--	--
Sum of positively identified compounds:			3.52	mg/m ³	

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%.

Table 4-2
Tank TY-103 Positively Identified Organic Compounds in TST Samples --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.040	0.015	38
2	Propanone (acetone)	67-64-1	0.042	0.010	23
3	1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.0032	0.0021	67
4	Propanenitrile	107-12-0	0.0088	0.0013	15
5	n-Hexane	110-54-3	0.0081	0.0011	14
6	Benzene	71-43-2	0.0047	0.0016	33
7	n-Butanenitrile	109-74-0	0.012	0.003	24
8	2-Pentanone	107-87-9	0.0047	0.0008	17
9	n-Heptane	142-82-5	0.0065	0.0008	13
10	Toluene	108-88-3	0.011	0.002	17
11	n-Pentanenitrile	110-59-8	0.0075	0.0008	10
12	2-Hexanone	591-78-6	0.0038	0.0007	19
13	n-Octane	111-65-9	0.0047	0.0007	15
14	n-Hexanenitrile	628-73-9	0.0061	0.0007	12
15	2-Heptanone	110-43-0	0.0034	0.0007	20
16	n-Nonane	111-84-2	0.0036	0.0007	20
17	n-Heptanenitrile	629-08-3	0.0045	0.0005	12
18	2-Octanone	111-13-7	0.0029	0.0007	24
19	n-Decane	124-18-5	0.0074	0.0013	18
20	n-Undecane	1120-21-4	0.044	0.012	27
21	n-Dodecane	112-40-3	0.81	0.19	24
22	n-Tridecane	629-50-5	4.00	1.32	33

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

² CAS = Chemical Abstract Service.

3 Average of 4 TST samples: 3 were 200 ml and 1 was 4-L.

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

Table 4-3

**Tank TY-103 Positively Identified Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹**

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Butanal ⁵	123-72-8	0.035	0.006	18
2	1-Butanol ⁵	71-36-3	0.15	0.04	25

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

2 CAS = Chemical Abstract Service.

3 Average of 4 TST samples: 3 were 200 ml and 1 was 4-L.

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

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

Table 4-4
Tank TY-103 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 (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.0032	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	< 0.0013	< 0.005	--
Propanone (acetone)	67-64-1	0.042	0.13	102
Ethanenitrile (acetonitrile)	75-05-8	0.040	0.075	61
Propanenitrile	107-12-0	0.0088	0.017	64
n-Butanenitrile	109-74-0	0.012	< 0.005	> 82
Benzene	71-43-2	0.0047	< 0.005	--
Toluene	108-88-3	0.011	0.013	17
n-Hexane	110-54-3	0.0081	0.38	192
n-Heptane	142-82-5	0.0065	0.006	8
n-Decane	124-18-5	0.0074	0.006	21

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 200 ml and 1 was 4-L.

3 Average of 3 samples.

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

Table 4-5
Tank TY-103 Tentatively Identified Organic Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard ³ Deviation (mg/m ³)
1	Propane	74-98-6	0.23	0.02
2	Methanol (methyl alcohol)	67-56-1	0.17	0.01
3	n-Butane	106-97-8	0.08	< 0.01
4	2-Propanol ⁴ (isopropyl alcohol)	67-63-0	0.06	< 0.01
5	3-Buten-2-one	78-94-4	< 0.03	--
6	1-Butanol	71-36-3	0.55	< 0.01
7	Pentanal	110-62-3	0.08	< 0.01
8	Hexanal	66-25-1	0.08	< 0.01
9	Nitric acid, butyl ester	928-45-0	0.05	< 0.01
10	Unknown Alcohol ⁵		0.08	--
11	Octanal	124-13-0	0.07	< 0.01
12	n-Undecane	1120-21-4	0.36	0.02
13	n-Dodecane	112-40-3	7.19	0.29
14	Undecane, 2,6-dimethyl-	17301-23-4	< 0.08	--
15	Unknown C12 Alkene/Cycloalkane		< 0.08	--
16	Unknown C14 Alkane		0.09	0.003
17	n-Tridecane	629-50-5	13.86	0.71
18	Unknown C12 Ketone		0.18	0.05
19	Unknown Alkane ⁵		0.05	--
20	n-Tetradecane	629-59-4	5.20	0.95
21	Unknown Ketone		0.09	0.05
Sum of tentatively identified compounds:			28.33	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples.

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

4 Detected in only 2 samples.

5 Detected in only 1 sample.

Table 4-6
Tank TY-103 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Methanol and Acetone		0.11	0.04
2	Ethanol	64-17-5	0.018	0.031
3	Trichloromonofluoromethane	75-69-4	0.12	0.003
4	2-Propanol (isopropyl alcohol)	67-63-0	0.011	0.018
5	1-Propanol	71-23-8	0.0099	0.0172
6	Pentanal	110-62-3	0.032	0.028
7	Hexanal	66-25-1	0.050	0.044
8	Tetrachloroethylene	127-18-4	0.056	0.005
9	Cyclotrisiloxane, hexamethyl	541-05-9	0.048	0.082
10	Heptanal	111-71-7	0.061	0.030
11	Cyclotetrasiloxane, octamethyl	556-67-2	0.027	0.046
12	Octanal	124-13-0	0.033	0.030
13	Nonanal	124-19-6	0.034	0.007
14	3-Dodecene, (E)-	7206-14-6	0.13	0.01
15	3-Dodecene, (E)-	7206-14-6	0.046	0.003
16	4-Dodecene	2030-84-4	0.031	0.006
17	Undecane, 2,6-dimethyl-	17301-23-4	0.069	0.006
18	Cyclohexane, hexyl	4292-75-5	0.058	0.007
19	Dodecane, 4-methyl-	6117-97-1	0.030	0.003
20	Undecane, 2,10-dimethyl-	17301-27-8	0.054	0.004
21	Tridecane, 7-methyl-	26730-14-3	0.15	0.01
22	4-Nonene, 5-butyl-	7367-38-6	0.081	0.140
23	1-Pentanol, 4-methyl-2-propyl	54004-41-0	0.012	0.020
24	Dodecane, 2,6,10-trimethyl	3891-98-3	0.0076	0.0132
25	4-Nonene, 5-butyl-	7367-38-6	0.030	0.027
26	4-Nonene, 5-butyl-	7367-38-6	0.032	0.055

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	5-Undecene, (E)-	764-97-6	0.031	0.054
28	6-Tridecene	24949-38-0	0.11	0.02
29	Decane and others		0.036	0.007
30	Cyclohexane, pentyl	4292-92-6	0.082	0.014
31	Tridecane, 2-methyl-	1560-96-9	0.046	0.009
32	Decane, 3,8-dimethyl-	17312-55-9	0.048	0.009
33	6-Dodecanone	6064-27-3	0.41	0.15
34	Cyclododecane, ethyl	28981-49-9	0.0088	0.0153
35	Cyclotetradecane	295-17-0	0.038	0.008
36	3-Dodecanone	1534-27-6	0.26	0.07
37	n-Tetradecane	629-59-4	14.72	2.00
38	Dodecane, 2,6,10-trimethyl	3891-98-3	0.046	0.012
39	6-Tridecanone	22026-12-6	0.88	0.29
40	3-Tridecanone	1534-26-5	0.62	0.19
41	n-Pentadecane	629-62-9	0.58	0.10
42	2-Tridecanone	593-08-8	0.54	0.29
43	1,1'-Biphenyl, 2-chloro-	2051-60-7	0.038	0.006
44	6-Dodecanone	6064-27-3	0.33	0.08
45	3-Tetradecanone	629-23-2	0.15	0.03
46	2-Tetradecanone	2345-27-9	0.11	0.02
47	Heptadecane 9-octyl	629-99-2	0.091	0.158
48	Benzenesulfonamide, N-butyl	3622-84-2	0.064	0.059
49	n-Hexadecane	544-76-3	0.53	0.92
50	Isopropyl Palmitate	142-91-6	0.017	0.029
51	2-Methyloctadecane	1560-88-9	0.30	0.52
Sum of tentatively identified compounds:			21.42	

1 CAS = Chemical Abstract Service.

WHC-SD-WM-ER-462 REV. 1

2 Average of 4 TST samples: 3 were 200 ml and 1 was 4-L, values listed are estimates.

Table 4-7
Tank TY-103 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
5	1-Propanol	71-23-8	0.0099	0.0172
23	1-Pentanol, 4-methyl-2-propyl	54004-41-0	0.012	0.020
43	1,1'-Biphenyl, 2-chloro-	2051-60-7	0.038	0.006
42	2-Tridecanone	593-08-8	0.54	0.29
51	2-Methyloctadecane	1560-88-9	0.30	0.52
46	2-Tetradecanone	2345-27-9	0.11	0.02
4	2-Propanol (isopropyl alcohol)	67-63-0	0.011	0.018
45	3-Tetradecanone	629-23-2	0.15	0.03
15	3-Dodecene, (E)-	7206-14-6	0.046	0.003
14	3-Dodecene, (E)-	7206-14-6	0.13	0.01
40	3-Tridecanone	1534-26-5	0.62	0.19
36	3-Dodecanone	1534-27-6	0.26	0.07
22	4-Nonene, 5-butyl-	7367-38-6	0.081	0.140
25	4-Nonene, 5-butyl-	7367-38-6	0.030	0.027
26	4-Nonene, 5-butyl-	7367-38-6	0.032	0.055
16	4-Dodecene	2030-84-4	0.031	0.006
27	5-Undecene, (E)-	764-97-6	0.031	0.054
39	6-Tridecanone	22026-12-6	0.88	0.29
33	6-Dodecanone	6064-27-3	0.41	0.15
44	6-Dodecanone	6064-27-3	0.33	0.08
28	6-Tridecene	24949-38-0	0.11	0.02
48	Benzenesulfonamide, N-butyl	3622-84-2	0.064	0.059
34	Cyclododecane, ethyl	28981-49-9	0.0088	0.0153
18	Cyclohexane, hexyl	4292-75-5	0.058	0.007
30	Cyclohexane, pentyl	4292-92-6	0.082	0.014
35	Cyclotetradecane	295-17-0	0.038	0.008

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
11	Cyclotetrasiloxane, octamethyl	556-67-2	0.027	0.046
9	Cyclotrisiloxane, hexamethyl	541-05-9	0.048	0.082
29	Decane and others		0.036	0.007
32	Decane, 3,8-dimethyl-	17312-55-9	0.048	0.009
19	Dodecane, 4-methyl-	6117-97-1	0.030	0.003
24	Dodecane, 2,6,10-trimethyl	3891-98-3	0.0076	0.0132
38	Dodecane, 2,6,10-trimethyl	3891-98-3	0.046	0.012
2	Ethanol	64-17-5	0.018	0.031
47	Heptadecane 9-octyl	7225-64-1	0.091	0.158
10	Heptanal	111-71-7	0.061	0.030
7	Hexanal	66-25-1	0.050	0.044
50	Isopropyl Palmitate	142-91-6	0.017	0.029
1	Methanol and Acetone		0.11	0.04
49	n-Hexadecane	544-76-3	0.53	0.92
41	n-Pentadecane	629-62-9	0.58	0.10
37	n-Tetradecane	629-59-4	14.72	2.00
13	Nonanal	124-19-6	0.034	0.007
12	Octanal	124-13-0	0.033	0.030
6	Pentanal	110-62-3	0.032	0.028
8	Tetrachloroethylene	127-18-4	0.056	0.005
3	Trichloromonofluoromethane	75-69-4	0.12	0.003
21	Tridecane, 7-methyl-	26730-14-3	0.15	0.01
31	Tridecane, 2-methyl-	1560-96-9	0.046	0.009
17	Undecane, 2,6-dimethyl-	17301-23-4	0.069	0.006
20	Undecane, 2,10-dimethyl-	17301-27-8	0.054	0.004
Sum of tentatively identified compounds:			21.42	

¹ CAS = Chemical Abstract Service.

WHC-SD-WM-ER-462 REV. 1

2 Average of 4 TST samples: 3 were 200 ml and 1 was 4-L, values listed are estimates.

Table 4-8
Tank TY-103 Tentatively Identified Organic Compounds in TST Samples
Sorted by Estimated Concentration --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
37	n-Tetradecane	629-59-4	14.72	2.00
39	6-Tridecanone	22026-12-6	0.88	0.29
40	3-Tridecanone	1534-26-5	0.62	0.19
41	n-Pentadecane	629-62-9	0.58	0.10
42	2-Tridecanone	593-08-8	0.54	0.29
49	n-Hexadecane	544-76-3	0.53	0.92
33	6-Dodecanone	6064-27-3	0.41	0.15
44	6-Dodecanone	6064-27-3	0.33	0.08
51	2-Methyloctadecane	1560-88-9	0.30	0.52
36	3-Dodecanone	1534-27-6	0.26	0.07
45	3-Tetradecanone	629-23-2	0.15	0.03
21	Tridecane, 7-methyl-	26730-14-3	0.15	0.01
14	3-Dodecene, (E)-	7206-14-6	0.13	0.01
3	Trichloromonofluoromethane	75-69-4	0.12	0.003
1	Methanol and Acetone		0.11	0.04
28	6-Tridecene	24949-38-0	0.11	0.02
46	2-Tetradecanone	2345-27-9	0.11	0.02
47	Heptadecane 9-octyl	7225-64-1	0.091	0.158
30	Cyclohexane, pentyl	4292-92-6	0.082	0.014
22	4-Nonene, 5-butyl-	7367-38-6	0.081	0.140
17	Undecane, 2,6-dimethyl-	17301-23-4	0.069	0.006
48	Benzenesulfonamide, N-butyl	3622-84-2	0.064	0.059
10	Heptanal	111-71-7	0.061	0.030
18	Cyclohexane, hexyl	4292-75-5	0.058	0.007
8	Tetrachloroethylene	127-18-4	0.056	0.005
20	Undecane, 2,10-dimethyl-	17301-27-8	0.054	0.004

WHC-SD-WM-ER-462 REV. 1

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
7	Hexanal	66-25-1	0.050	0.044
9	Cyclotrisiloxane, hexamethyl	541-05-9	0.048	0.082
32	Decane, 3,8-dimethyl-	17312-55-9	0.048	0.009
15	3-Dodecene, (E)-	7206-14-6	0.046	0.003
31	Tridecane, 2-methyl-	1560-96-9	0.046	0.009
38	Dodecane, 2,6,10-trimethyl	3891-98-3	0.046	0.012
35	Cyclotetradecane	295-17-0	0.038	0.008
43	1,1'-Biphenyl, 2-chloro-	2051-60-7	0.038	0.006
29	Decane and others		0.036	0.007
13	Nonanal	124-19-6	0.034	0.007
12	Octanal	124-13-0	0.033	0.030
6	Pentanal	110-62-3	0.032	0.028
26	4-Nonene, 5-butyl-	7367-38-6	0.032	0.055
27	5-Undecene, (E)-	764-97-6	0.031	0.054
16	4-Dodecene	2030-84-4	0.031	0.006
25	4-Nonene, 5-butyl-	7367-38-6	0.030	0.027
19	Dodecane, 4-methyl-	6117-97-1	0.030	0.003
11	Cyclotetrasiloxane, octamethyl	556-67-2	0.027	0.046
2	Ethanol	64-17-5	0.018	0.031
50	Isopropyl Palmitate	142-91-6	0.017	0.029
23	1-Pentanol, 4-methyl-2-propyl	54004-41-0	0.012	0.020
4	2-Propanol (isopropyl alcohol)	67-63-0	0.011	0.018
5	1-Propanol	71-23-8	0.0099	0.0172
34	Cyclododecane, ethyl	28981-49-9	0.0088	0.0153
24	Dodecane, 2,6,10-trimethyl	3891-98-3	0.0076	0.0132
Sum of tentatively identified compounds:			21.42	

¹ CAS = Chemical Abstract Service.

² Average of 4 TST samples: 3 were 200 ml and 1 was 4-L, values listed are estimates.