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Title/Desc:

TANK 241TY104 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED
IN 4/1995

COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

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ECN

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Page 2 of 2

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

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15. Design Verification Required

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16. Cost Impact

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SDD/DD	☐	Seismic/Stress Analysis	☐	Tank Calibration Manual	☐
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	☐
Environmental Report	☐	Inspection Plan	☐		☐
Environmental Permit	☐	Inventory Adjustment Request	☐		☐

19. Other Affected Documents: (NOTE: Documents listed below will not be revised by this ECN.) Signatures below indicate that the signing organization has been notified of other affected documents listed below.

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Cog. Mgr. T. J. Kelley <i>TJ Kelley</i>	<u>9/25/95</u>	QA	
QA		Safety	
Safety		Design	
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APPROVED FOR PUBLIC RELEASE

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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.

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Tank 241-TY-104 Headspace Gas and Vapor Characterization Results for Samples Collected in April 1995

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Date Published
September 1995

Prepared for the U.S. Department of Energy
Office of Environmental Restoration and
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Hanford Company

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**Tank 241-TY-104 Headspace Gas and Vapor Characterization Results
for Samples Collected in April 1995**

September 14, 1995

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Acronyms and Abbreviations

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

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**Tank 241-TY-104 Headspace Gas and Vapor Characterization Results
for Samples Collected in April 1995**

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank TY-104 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). The tank TY-104 headspace was sampled 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 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). However, current governing operating specifications for single shell Watchlist waste tanks, such as tank TY-104, specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995a).

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

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

1.3 Sampling Overview

Tank TY-104 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 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 understood (Huckaby 1994a), and until the ISS method has been validated and the discrepancies resolved, results from early ISS events should be considered suspect. Only results from the April 1995 VSS sampling event are discussed here. The ISS event sampling information is reported by Pingel (1994) and Mahon (1995). Jenkins et al. (1995a) and Ligoŕke et al. (1995) report analytical results for the August 1994 ISS event.

Headspace samples discussed in this report are thought to have been representative of tank TY-104 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 as to how the tank TY-104 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-104 is the first tank in a 3-tank cascade with tanks TY-105 and TY-106. It is connected to tank TY-105 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long cascade line. Tanks TY-105 and TY-106 are connected by a similar line. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank TY-105 or tank TY-106 may be transferred to tank TY-104 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for either tanks TY-105 or TY-106 to assess their potential effect on tank TY-104.

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

2.0 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank TY-104 using the VSS on April 27, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-TY-104 Tank Characterization Plan* (Homi 1995). The tank headspace temperature was determined to be 15.6 °C. Air from the tank TY-104 headspace was withdrawn from a single elevation via the temperature/vapor probe mounted in riser 3, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 40°C. All tank air samples were collected between 10:29 a.m. and 3:53 p.m., with no sampling anomalies noted.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL). The 40 tank air samples and 2 ambient air control samples collected are listed in Table 2-1 by analytical laboratory. Table 2-1 also lists the 14 trip blanks and 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 canisters were prepared and analyzed by PNL (Klinger et al. 1995a).

Analyses of the inorganic sorbent traps were performed within 8 days of sample collection, and analyses of SUMMATM canisters for inorganic compounds were performed within 7 days after sample collection (Ligotke 1995). This fulfilled 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. PNL results were produced at PNL quality assurance impact level 2.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

The concentration of ammonia in the headspace of TY-103 was measured at 61 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 61 ppmv corresponds to less than 0.05 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank TY-104 was determined to be < 49 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 49 ppmv hydrogen concentration in tank TY-104 would correspond to about 0.12 % of its LFL. At this level, hydrogen is not a flammability concern in tank TY-104.

The reported nitrous oxide concentration in tank TY-104, 98 ppmv, is typical of other waste tanks that have been sampled. 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 1995b), and as high as 878 ppmv in tank U-103 (Ligotke et al. 1995). Under proper conditions, nitrous oxide can serve as an oxidizer to support combustion. However, Cashdollar et al. (1992) found that nitrous oxide had no significant effect on the flammability of hydrogen and air mixtures for hydrogen concentrations less than 20 vol%, and that "small amounts of nitrous oxide (relative to air) do not appear to have much effect on the flammability". Their results suggest the measured nitrous oxide concentration is much too low to have a significant effect on the flammability of the tank TY-104 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank TY-104 headspace was measured in each of the 3 SUMMATM canister samples to be < 23 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

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

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-104 headspace, measured to be < 23 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-104 April 1995 sampling event, for example, were measured to have an average 371 ppmv of carbon dioxide.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank TY-104 headspace were determined to be 0.18 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-104. 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-104 headspace.

The water vapor concentration of tank TY-104 was determined to be about 12.8 mg/L, at the measured tank headspace temperature of 15.6 °C and pressure of 982.3 mbar (736.9 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 15.7 mbar (11.8 torr), to a dew point of 13.7 °C, and to a relative humidity of 88 %.

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water vapor, the most abundant waste constituents in the tank TY-104 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces sampled to date and, along with hydrogen, are usually the dominant 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 very good for the methods used. Relative standard deviations range from 1.2 % for water vapor to

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.

about 11 % for nitric oxide results. The relatively poor precision of the nitric oxide results is probably due to the variable levels of background contamination in the sorbent traps. 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 indicate proper control was maintained both in the field and in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank TY-104 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. PNL and ORNL both used gas chromatographs (GCs) equipped with mass spectrometer (MS) detectors to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995b) and Klinger et al. (1995a).

SUMMA™ sample results produced by PNL should be considered to be the primary organic vapor data for tank TY-104. These results were produced at PNL quality assurance impact level 2, and all PNL analyses were completed within 8 days after sample collection, well within 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. 1995b). 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 from 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 (Klinger et al. 1995a). Only 3 of the 39 TO-14 target analytes (trichlorofluoromethane, 1,1,2-trichloro-1,2,2-trifluoroethane, and tetrachloromethane) and only 5 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. (1995b) reported 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, only 6 of the 24 compounds positively identified by ORNL were measured to be within the calibration range of the instrument in all 3 TST samples. The average concentrations of the positively identified compounds, from the analysis of 3 TSTs, are given in Tables 4-2, 4-3, and 4-4. Table 4-2 lists the positively identified, quantitated analytes, Table 4-3 lists the positively identified analytes which were not quantitated (because the measurement was outside the calibration range for at least 1 sample), and Table 4-4 lists the positively identified analytes which exceeded their practical holding times. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these 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 a practical holding time for butanal of only 1 day. 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-104 and obtain concentration in ppmv of analyte in moist tank air, multiply the dry-air ppmv concentrations by 0.984.

Eleven target analytes were common to both TST and SUMMATM analyses. Table 4-5 lists these, and their reported average concentrations in TST and SUMMATM samples. Results from these 2 sampling and analytical methods are in fairly good agreement. As indicated in Table 4-5, the reported concentrations of propanone, ethanenitrile, and propanenitrile are quite similar in SUMMATM and TST samples. Other target analytes are generally only present at very low concentrations, and none are near levels of concern.

Propanone and n-tridecane are the only organic target analytes measured above 0.1 ppmv. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

4.2 Tentatively Identified Organic Compounds

In addition to the target analytes, the ORNL and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and may also determine its molecular weight. The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Using this method, many analytes can be tentatively identified with reasonable confidence without having to inject 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 SUMMATM samples. Analyses of the samples are designed to recover, separate, identify, and quantify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (e.g., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (e.g., butanal) from SUMMATM samples has been problematic.

The tentatively identified compounds recovered from SUMMA™ samples, in the order by which the eluted chromatographically, are given in Table 4-6 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 4-7. 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 (Table 4-7) is rather long and finding any given compound may be difficult, the list has been sorted both alphanumerically by compound name (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. (1995b) and Klinger et al. (1995a), respectively, and should be reviewed before this data are used for decision making. Concentrations given in Tables 4-6 through 4-9 should be considered rough estimates.

4.3 Discussion of Organic Compounds

The organic compounds listed in Tables 4-1 through 4-7 may be classified as either 1) organic compounds added to tank TY-104 as waste that are still evaporating, or 2) organic compounds that have been generated by reactions of the original waste.

Organic vapors 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 15 % of the total estimated organic vapor in tank TY-104 TST samples is due to n-dodecane, n-tridecane, and n-tetradecane.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 48 and 77 in Table 4-7) may also have been sent to tank TY-104 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-104 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-104 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-104 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-104, including dichlorofluoromethane, trichlorofluoromethane (which is frequently detected in the waste tanks), trichloromethane, tetrachloromethane, 1,1,1-trichloroethane, 1,1,2-trichloro-1,2,2-trifluoroethane, and tetrachloroethene. The less volatile of these compounds are frequently used as cleaning solvents and may have been sent to the waste tanks when they became radiologically contaminated. The more volatile halocarbons, dichlorofluoromethane and trichlorofluoromethane, may be associated with the urethane foam that was used to seal tank concrete pit covers.

Also present in the TST samples from tank TY-104 are several chlorinated and polychlorinated biphenyls (PCBs), (i.e., Cmpd # 160, 166, 168, 171-175, 178, 180-184, and 186 in Table 4-7). These are conveniently grouped together in Table 4-8. As indicated in Table 4-9, 8 of the 15 chlorinated biphenyls had average estimated concentrations above 0.001 mg/m³ in TST samples. PCBs were used for various industrial purposes, and small quantities may have been sent to the waste tanks when contaminated..

Organic vapors in the second category, those that have been generated via radiolytic and chemical reactions of the waste, constitute the majority of compounds listed in Tables 4-1 through 4-9. This category includes the alcohols, aldehydes, alkenes, alkyl nitrates, alkyl nitrites, 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-104 was estimated by Jenkins et al. (1995b) to be about 3 mg/m³ from the analysis of 3 TST samples by GC/MS. A similar summation of organic compounds measured in SUMMATM samples from tank TY-104 provides an estimated total organic vapor concentration of 1.5 mg/m³. Compared to other waste tanks that have been sampled, tank TY-104 has a relatively low concentration of organic vapors.

5.0 SUMMARY

The tank TY-104 headspace was sampled in April 1995 for gases and vapors to address flammability and industrial hygiene concerns. Collection and analysis of samples has been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995).

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Table 2-1
Tank TY-104 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	4.0	Organic vapors	6 tank air samples
		6.0	Organic vapors	6 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-104 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	61	2	3
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	< 23	--	--
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 23	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 49	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.18	0.02	11
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	98	2.3	2
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	15,900 (11.8 mg/L)	200 (0.1 mg/L)	1.2

¹ CAS = Chemical Abstracts Service.

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

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

Cmpd #	Compound	CAS ¹ Number	Average ² (ppmv)	Standard Deviation (ppmv)	RSD ³ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.069	0.009	13
2	Propanone (acetone)	67-64-1	0.11	0.01	11
3	Trichlorofluoromethane	75-69-4	0.032	0.003	10
4	1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	0.022	0.002	10
5	Propanenitrile	107-12-0	0.017	0.010	56
6	1-Propanol	71-23-8	0.009	0.005	51
7	2-Butanone	78-93-3	0.007	0.0004	6
8	Tetrachloromethane (carbon tetrachloride)	56-23-5	0.009	0.0004	4
9	Methane	74-82-8	< 23	--	--
Sum of positively identified compounds:			0.95	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-104 Quantitatively Measured Organic Compounds in TST Samples --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.043	0.006	13
2	Propanenitrile	107-12-0	0.010	0.001	6
3	n-Butanenitrile	109-74-0	0.0061	0.0005	8
4	2-Pentanone	107-87-9	0.0024	0.0001	3
5	n-Pentanenitrile	110-59-8	0.0014	0.00002	1
6	n-Undecane	1120-21-4	0.0012	0.0001	9

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 6-L TST samples.

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

Table 4-3
Tank TY-104 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	Propanone (acetone)	67-64-1	0.097	0.009	9
2	1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.00016	0.00001	8
3	n-Hexane	110-54-3	0.00069	0.00006	9
4	Benzene	71-43-2	0.00037	0.00001	3
5	1-Butanol	71-36-3	0.042	0.003	6
6	n-Heptane	142-82-5	0.00042	0.00003	6
7	Toluene	108-88-3	0.00058	0.00003	5
8	2-Hexanone	591-78-6	0.00081	0.00006	8
9	n-Octane	111-65-9	0.00019	0.00001	7
10	n-Hexanenitrile	628-73-9	0.00074	0.00003	4
11	2-Heptanone	110-43-0	0.00074	0.00002	3
12	n-Nonane	111-84-2	0.00021	0.00002	8
13	n-Heptanenitrile	629-08-3	0.00052	0.00003	5
14	2-Octanone	111-13-7	0.00041	0.00002	6
15	n-Decane	124-18-5	0.00029	0.00003	9
16	n-Dodecane	112-40-3	0.016	0.001	7
17	n-Tridecane	629-50-5	0.12	0.002	2

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, 6-L TST samples.

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

Table 4-4
Tank TY-104 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	0.036	0.002	5

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 6-L TST samples.

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

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

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

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	PRD ⁴ (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.00016	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	< 0.00089	< 0.005	--
Propanone (acetone)	67-64-1	0.097	0.11	12
Ethanenitrile (acetonitrile)	75-05-8	0.043	0.069	46
Propanenitrile	107-12-0	0.010	0.017	52
n-Butanenitrile	109-74-0	0.0061	< 0.005	> 20
Benzene	71-43-2	0.00037	< 0.005	--
Toluene	108-88-3	0.00058	< 0.005	--
n-Hexane	110-54-3	0.00069	< 0.005	--
n-Heptane	142-82-5	0.00042	< 0.005	--
n-Decane	124-18-5	0.00029	< 0.005	--

1 CAS = Chemical Abstract Service.

2 Average of 3, 6-L TST samples.

3 Average of 3 samples.

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

Table 4-6
Tank TY-104 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	Methyl nitrite	624-91-9	0.21	0.06
2	Methanol (methyl alcohol)	67-56-1	0.14	0.02
3	Unknown alkyl nitrate		0.06	0.01
4	1-Butanol	71-36-3	0.10	0.01
5	n-Tridecane	629-50-5	0.06	< 0.01
Sum of tentatively identified compounds:			0.57	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples, presented values are estimates.

Table 4-7
Tank TY-104 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	1-Propene, 2-methyl-	115-11-7	0.0040	0.0015
2	Methyl alcohol and others		0.036	0.032
3	Ethylene Oxide	75-21-8	0.017	0.030
4	1-Propene, 2-methyl-	115-11-7	0.0042	0.0005
5	Hydrazine, 1,1-dimethyl	57-14-7	0.0031	0.0006
6	Methane, dichlorofluoro-	75-43-4	0.0017	0.0002
7	Ethanol	64-17-5	0.026	0.003
8	Trichlorofluoromethane	75-69-4	0.038	0.006
9	Silane, chlorotrimethyl	75-77-4	0.00095	0.00165
10	Isopropyl Alcohol	67-63-0	0.0071	0.0011
11	Cyclopropane, ethyl	1191-96-4	0.00042	0.00072
12	Ethane, 1,1,2-trichloro- 1,2,2-trifluoro-	76-13-1	0.11	0.01
13	Methyl nitrate	598-58-3	0.031	0.002
14	2-Propen-1-ol	107-18-6	0.00059	0.00051
15	Pentane, 2-methyl-	107-83-5	0.0012	0.0001
16	1-Propanol	71-23-8	0.026	0.002
17	3-Buten-2-one	78-94-4	0.0024	0.0004
18	2-Butanone	78-93-3	0.018	0.002
19	Chloroform	67-66-3	0.0045	0.0007
20	Nitric acid, ethyl ester	625-58-1	0.031	0.002
21	Furan, tetrahydro-	109-99-9	0.0029	0.0008
22	1-Propanol, 2-methyl-	78-83-1	0.0013	0.0001
23	Acetic acid	64-19-7	0.00061	0.00106
24	Ethane, 1,1,1-trichloro	71-55-6	0.00067	0.00058
25	3-Pentanol, 2-methyl-	565-67-3	0.00066	0.00059
26	Propanenitrile, 2,2-dimethyl	630-18-2	0.0022	0.0013

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	2-Butenal	4170-30-3	0.0022	0.0015
28	2-Butanone, 3-methyl	563-80-4	0.0015	0.0017
29	1,4-Butanediamine	110-60-1	0.00080	0.00076
30	Nitric acid, 1-methylethyl ester	1712-64-7	0.0046	0.0002
31	Pentanal	110-62-3	0.011	0.001
32	Isopropyl Alcohol	67-63-0	0.0010	0.0009
33	2-Heptene, (E)-	14686-13-6	0.00046	0.00080
34	1H-Imidazole, 2-methyl-	693-98-1	0.0016	0.0002
35	Nitric acid, propyl ester	627-13-4	0.027	0.001
36	3-Buten-2-one, 3-methyl-	814-78-8	0.0014	0.0002
37	Pyrazine	290-37-9	0.0025	0.0002
38	Propane, 2-methyl-2-nitro-	594-70-7	0.0060	0.0002
39	3-Pentanone, 2-methyl-	565-69-5	0.00076	0.00018
40	1-Pentanol	71-41-0	0.0023	0.0041
41	2-Pentanone, 3-methyl-	565-61-7	0.00037	0.00032
42	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0019	0.0001
43	3-Hexanone	589-38-8	0.00070	0.00003
44	cis-1-nitro-1-propene	27675-36-1	0.0080	0.0006
45	1-butanamine, N-ethylidene	6898-74-4	0.0030	0.0004
46	Hexanal	66-25-1	0.0092	0.0006
47	Tetrachloroethylene	127-18-4	0.024	0.001
48	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0023	0.0011
49	Nitric acid, butyl ester	928-45-0	0.011	0.0003
50	Pyridine, 3-methyl-	108-99-6	0.0023	0.0004
51	1-Hexene, 4,5-dimethyl-	16106-59-5	0.00020	0.00034
52	Acetamide, N-methyl-	79-16-3	0.00040	0.00070
53	4-Heptanone	123-19-3	0.00022	0.00039
54	2-Hexenal, (E)-	6728-26-3	0.0013	0.0005

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Nitric acid, propyl ester and ethylbenzene		0.0014	0.0003
56	1-Hexanol	111-27-3	0.0055	0.0004
57	p-Xylene	106-42-3	0.00046	0.00043
58	Propane, 2-[(1,1-dimethylethyl) sulfonyl]-2-methyl-	1886-75-5	0.0023	0.0007
59	3-Heptanone	106-35-4	0.0067	0.0003
60	2-Nonene, (E)-	6434-78-2	0.00043	0.00039
61	3-Heptanol	589-82-2	0.0036	0.0003
62	Heptanal	111-71-7	0.0088	0.0005
63	Acetonitrile, hydroxy-	107-16-4	0.00096	0.00166
64	Pyridine, 2-ethyl-	100-71-0	0.00022	0.00039
65	trans-3,4-Dimethylcyclopentanone	19550-73-3	0.00021	0.00037
66	Pentanol, 5-amino	2508-29-4	0.0020	0.0017
67	Nitric acid, pentyl ester	1002-16-0	0.0054	0.0003
68	Propane, 2-ethoxy-2-methyl-	637-92-3	0.00036	0.00062
69	2,3-Dimethyl-2-hexanol	1955-03-9	0.00022	0.00038
70	2-Pentene, 2,4-dimethyl-	625-65-0	0.0010	0.0002
71	2-Pentanol, 2,3-dimethyl-	4911-70-0	0.00087	0.00011
72	2-Heptanone, 6-methyl-	928-68-7	0.0068	0.0003
73	3-Tetradecene, (E)-	41446-68-8	0.00093	0.00010
74	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	0.0013	0.0001
75	1-Hexene, 5,5-dimethyl-	7116-86-1	0.0023	0.0003
76	1-Heptanol	111-70-6	0.0053	0.0005
77	Cyclotetrasiloxane, octamethyl	556-67-2	0.0013	0.0013
78	Octanal	124-13-0	0.0068	0.0007
79	5-Decene (E)	7433-56-9	0.0011	0.0001
80	Decane, 4-methyl-	2847-72-5	0.00071	0.000003
81	Nitric acid, hexyl ester	20633-11-8	0.0040	0.0003
82	Hexane, 2,5-dimethyl-	592-13-2	0.0021	0.0002

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
83	Cyclopentane, 1-ethyl-3-methyl-	2613-66-3	0.00039	0.00034
84	Nitric acid, pentyl ester	1002-16-0	0.00031	0.00054
85	Cyclohexanone, 2,2,6-trimethyl	2408-37-9	0.00035	0.00031
86	1-Propanol, 2,2-dimethyl nitrate	926-42-1	0.0036	0.0004
87	5-Undecene	4941-53-1	0.0010	0.0001
88	1-Decanol, 2-ethyl	21078-65-9	0.00095	0.00009
89	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.0022	0.0001
90	1-Octanol	111-87-5	0.0029	0.0001
91	Acetophenone	98-86-2	0.0028	0.00003
92	Octanenitrile	124-12-9	0.0024	0.0001
93	1-Decene, 5-methyl-	54244-79-0	0.0019	0.0001
94	2-Nonanone	821-55-6	0.0022	0.0002
95	Benzene, nitro-	98-95-3	0.0037	0.0002
96	Nonanal	124-19-6	0.0056	0.0008
97	2-Undecene, (Z)-	821-96-5	0.00060	0.00008
98	Nonane, 3-methyl-5-propyl-	31081-18-2	0.00092	0.00015
99	Nitric acid, hexyl ester	20633-11-8	0.0029	0.0004
100	2-Hexanone, 6-methoxy-	29006-00-6	0.00044	0.00039
101	Benzoic acid, 2-[(trimethylsilyl)oxy]-trimethyl	3789-85-3	0.00028	0.00048
102	n-Amylcyclohexane	4292-92-6	0.0011	0.0002
103	Heptane, 3-ethyl-2-methyl-	14676-29-0	0.0014	0.0006
104	Undecane, 2-methyl-	7045-71-8	0.00075	0.00008
105	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	0.0034	0.0005
106	1-Nonanol	143-08-8	0.0019	0.0004
107	3-Dodecene, (E)-	7206-14-6	0.0069	0.0005
108	2-Decanone	693-54-9	0.0032	0.0001
109	1-Decene	872-05-9	0.0013	0.0001
110	Undecane, 2,6-dimethyl-	17301-23-4	0.0025	0.0002

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
111	Benzene, 1-methyl-3-nitro-	99-08-1	0.0012	0.0001
112	Nitric acid, nonyl ester	20633-13-0	0.0014	0.0003
113	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.0010	0.00003
114	Nonadecane, 9-methyl-	13287-24-6	0.00019	0.00032
115	Cyclohexane, hexyl	4292-75-5	0.0019	0.0001
116	Dodecane, 4-methyl-	6117-97-1	0.00087	0.00001
117	Undecane, 2,10-dimethyl-	17301-27-8	0.0015	0.0001
118	Tridecane, 7-methyl-	26730-14-3	0.0046	0.0001
119	2(3H)-Furanone, 5-butyldihydro-	104-50-7	0.0041	0.0005
120	Furan, tetrahydro-2, 5-dipropyl-	4457-62-9	0.0020	0.0003
121	4-Nonene, 5-butyl- and others		0.0017	0.0003
122	7-Tetradecene, (Z)-	41446-60-0	0.0025	0.0002
123	Undecanenitrile	2244-07-7	0.0015	0.0013
124	2-Pyrrolidinone	616-45-5	0.00053	0.00091
125	6-Tridecene	24949-38-0	0.0012	0.0003
126	1-Ethylpropyl octanoate and others		0.00023	0.00041
127	Pyridine, 2,3,6-trimethyl	1462-84-6	0.00043	0.00037
128	1-Methyl-2-(4-methylpentyl)-cyclopentane		0.00018	0.00032
129	Cyclohexanol, 4-methyl- 1-(1-methylethyl)-	470-65-5	0.00018	0.00032
130	5-Decanone	820-29-1	0.00098	0.00005
131	Undecane, 3-ethyl-	17312-58-2	0.0016	0.0014
132	n-Amylcyclohexane	29949-27-7	0.00072	0.00124
133	Nonane, 4,5-dimethyl-	17302-23-7	0.0016	0.00001
134	1-Pyrrolidinecarboxaldehyde	3760-54-1	0.00040	0.00035
135	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl	40702-26-9	0.0050	0.0003
136	6-Dodecanone	6064-27-3	0.023	0.005
137	2(3H)-Furanone, 5-heptyldihydro- and others		0.0057	0.0015

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
138	Furan, tetrahydro-2, 5-dipropyl-	4457-62-9	0.0048	0.0011
139	2,2'-Bioxepane	74793-02-5	0.0069	0.0002
140	3-Dodecanone	1534-27-6	0.019	0.004
141	Tetradecane	629-59-4	0.30	0.01
142	Decanamide, N-(2-hydroxyethyl)-	7726-08-1	0.0036	0.0032
143	Dodecanamide, N-(2-hydroxyethyl)-	142-78-9	0.0026	0.0045
144	1-Methylcycloheptanol	3761-94-2	0.0010	0.0008
145	Tridecane, 5-methyl-	25117-31-1	0.00070	0.00004
146	Hexadecane	544-76-3	0.0034	0.0002
147	3-Hexyne-2,5-diol, 2,5-dimethyl-	142-30-3	0.0023	0.0008
148	6-Tridecanone	22026-12-6	0.019	0.001
149	4-Dodecanone, 11-methyl	29366-35-6	0.0084	0.0146
150	Cyclohexene, 1-methyl-3-(1-methylethyl)-	13828-31-4	0.0018	0.0031
151	Cyclohexanol, 4-methyl-1-(1-methylethyl)-	470-65-5	0.0011	0.0010
152	3-Tridecanone	1534-26-5	0.038	0.006
153	Pentadecane	629-62-9	0.013	0.003
154	2-Tridecanone	593-08-8	0.011	0.003
155	3-Dodecanol	10203-30-2	0.0028	0.0049
156	2-Decanol	1120-06-5	0.0048	0.0014
157	2-Undecanol	1653-30-1	0.0012	0.0020
158	(S)-1-Amino-2-(methoxymethyl)-pyrrolidine	59983-39-0	0.00060	0.00104
159	Alkyl cyclohexane		0.00092	0.00025
160	1,1'-Biphenyl, 4-chloro	2051-62-9	0.0023	0.0001
161	4-Decanone	624-16-8	0.013	0.001
162	4-Tetradecanone	26496-20-8	0.013	0.0003
163	3-Dodecanone	1534-27-6	0.0055	0.0096
164	3-Tetradecanone	629-23-2	0.012	0.010
165	2-Tetradecanone	2345-27-9	0.0057	0.0003

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
166	1,1'-Biphenyl, 4-chloro	2051-62-9	0.00049	0.00044
167	Diethyl Phthalate	84-66-2	0.00061	0.00053
168	1,1'-Biphenyl, 2,2'-dichloro-	13029-08-8	0.0012	0.0001
169	Pentadecane	629-62-9	0.00022	0.00038
170	2-Heptadecanone	2922-51-2	0.00018	0.00031
171	1,1'-Biphenyl, 2,5-dichloro-	34883-39-1	0.00099	0.00006
172	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.0020	0.0002
173	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.0014	0.0002
174	1,1'-Biphenyl, 2,3-dichloro-	16605-91-7	0.0011	0.0003
175	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.00066	0.00114
176	Isopropyl Myristate	110-27-0	0.00043	0.00075
177	Benzenesulfonamide, N-butyl	3622-84-2	0.0023	0.0023
178	1,1'-Biphenyl, 2,4',5-trichloro-	16606-02-3	0.0038	0.0009
179	Hexadecane, 7,9-dimethyl-	21164-95-4	0.00071	0.00020
180	1,1'-Biphenyl, 2,4,4'-trichloro-	7012-37-5	0.0026	0.0006
181	1,1'-Biphenyl, 2,3,4-trichloro-	55702-46-0	0.00091	0.00030
182	1,1'-Biphenyl, 2,3,4-trichloro-	55702-46-0	0.00094	0.00012
183	1,1'-Biphenyl, 2,3,3',5'-tetrachloro-	41464-49-7	0.0028	0.0002
184	1,1'-Biphenyl, 2,3,4',6-tetrachloro-	52663-58-8	0.00020	0.00034
185	Isopropyl Palmitate	142-91-6	0.00067	0.00065
186	Tetrachlorobiphenyl and others		0.00018	0.00031
Sum of tentatively identified compounds:			1.23	

1 CAS = Chemical Abstract Service.

2 Average of 3, 6-L TST samples, presented values are estimates.

Table 4-8
Tank TY-104 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)
158	(S)-1-Amino-2-(methoxymethyl)-pyrrolidine	59983-39-0	0.00060	0.00104
1	1-Propene, 2-methyl-	115-11-7	0.0040	0.0015
51	1-Hexene, 4,5-dimethyl-	16106-59-5	0.00020	0.00034
4	1-Propene, 2-methyl-	115-11-7	0.0042	0.0005
86	1-Propanol, 2,2-dimethyl nitrate	926-42-1	0.0036	0.0004
76	1-Heptanol	111-70-6	0.0053	0.0005
126	1-Ethylpropyl octanoate and others		0.00023	0.00041
75	1-Hexene, 5,5-dimethyl-	7116-86-1	0.0023	0.0003
40	1-Pentanol	71-41-0	0.0023	0.0041
88	1-Decanol, 2-ethyl	21078-65-9	0.00095	0.00009
128	1-Methyl-2-(4-methylpentyl)-cyclopentane		0.00018	0.00032
134	1-Pyrrolidinecarboxaldehyde	3760-54-1	0.00040	0.00035
90	1-Octanol	111-87-5	0.0029	0.0001
45	1-butanamine, N-ethylidene	6898-74-4	0.0030	0.0004
109	1-Decene	872-05-9	0.0013	0.0001
16	1-Propanol	71-23-8	0.026	0.002
106	1-Nonanol	143-08-8	0.0019	0.0004
56	1-Hexanol	111-27-3	0.0055	0.0004
93	1-Decene, 5-methyl-	54244-79-0	0.0019	0.0001
144	1-Methylcycloheptanol	3761-94-2	0.0010	0.0008
22	1-Propanol, 2-methyl-	78-83-1	0.0013	0.0001
174	1,1'-Biphenyl, 2,3-dichloro-	16605-91-7	0.0011	0.0003
175	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.00066	0.00114
178	1,1'-Biphenyl, 2,4',5-trichloro-	16606-02-3	0.0038	0.0009
180	1,1'-Biphenyl, 2,4,4'-trichloro-	7012-37-5	0.0026	0.0006
173	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.0014	0.0002

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
181	1,1'-Biphenyl, 2,3,4-trichloro-	55702-46-0	0.00091	0.00030
182	1,1'-Biphenyl, 2,3,4-trichloro-	55702-46-0	0.00094	0.00012
183	1,1'-Biphenyl, 2,3,3',5'-tetrachloro-	41464-49-7	0.0028	0.0002
172	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.0020	0.0002
171	1,1'-Biphenyl, 2,5-dichloro-	34883-39-1	0.00099	0.00006
184	1,1'-Biphenyl, 2,3,4',6-tetrachloro-	52663-58-8	0.00020	0.00034
160	1,1'-Biphenyl, 4-chloro	2051-62-9	0.0023	0.0001
166	1,1'-Biphenyl, 4-chloro	2051-62-9	0.00049	0.00044
168	1,1'-Biphenyl, 2,2'-dichloro-	13029-08-8	0.0012	0.0001
29	1,4-Butanediamine	110-60-1	0.00080	0.00076
34	1H-Imidazole, 2-methyl-	693-98-1	0.0016	0.0002
170	2-Heptadecanone	2922-51-2	0.00018	0.00031
28	2-Butanone, 3-methyl	563-80-4	0.0015	0.0017
27	2-Butenal	4170-30-3	0.0022	0.0015
41	2-Pentanone, 3-methyl-	565-61-7	0.00037	0.00032
42	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0019	0.0001
33	2-Heptene, (E)-	14686-13-6	0.00046	0.00080
18	2-Butanone	78-93-3	0.018	0.002
14	2-Propen-1-ol	107-18-6	0.00059	0.00051
165	2-Tetradecanone	2345-27-9	0.0057	0.0003
124	2-Pyrrolidinone	616-45-5	0.00053	0.00091
154	2-Tridecanone	593-08-8	0.011	0.003
72	2-Heptanone, 6-methyl-	928-68-7	0.0068	0.0003
156	2-Decanol	1120-06-5	0.0048	0.0014
71	2-Pentanol, 2,3-dimethyl-	4911-70-0	0.00087	0.00011
157	2-Undecanol	1653-30-1	0.0012	0.0020
60	2-Nonene, (E)-	6434-78-2	0.00043	0.00039
54	2-Hexenal, (E)-	6728-26-3	0.0013	0.0005

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
100	2-Hexanone, 6-methoxy-	29006-00-6	0.00044	0.00039
108	2-Decanone	693-54-9	0.0032	0.0001
70	2-Pentene, 2,4-dimethyl-	625-65-0	0.0010	0.0002
97	2-Undecene, (Z)-	821-96-5	0.00060	0.00008
94	2-Nonanone	821-55-6	0.0022	0.0002
139	2,2'-Bioxepane	74793-02-5	0.0069	0.0002
69	2,3-Dimethyl-2-hexanol	19550-03-9	0.00022	0.00038
137	2(3H)-Furanone, 5-heptyldihydro- and others		0.0057	0.0015
119	2(3H)-Furanone, 5-butyldihydro-	104-50-7	0.0041	0.0005
105	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	0.0034	0.0005
89	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.0022	0.0001
74	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	0.0013	0.0001
152	3-Tridecanone	1534-26-5	0.038	0.006
61	3-Heptanol	589-82-2	0.0036	0.0003
59	3-Heptanone	106-35-4	0.0067	0.0003
43	3-Hexanone	589-38-8	0.00070	0.00003
164	3-Tetradecanone	629-23-2	0.012	0.010
163	3-Dodecanone	1534-27-6	0.0055	0.0096
73	3-Tetradecene, (E)-	41446-68-8	0.00093	0.00010
155	3-Dodecanol	10203-30-2	0.0028	0.0049
39	3-Pentanone, 2-methyl-	565-69-5	0.00076	0.00018
107	3-Dodecene, (E)-	7206-14-6	0.0069	0.0005
17	3-Buten-2-one	78-94-4	0.0024	0.0004
147	3-Hexyne-2,5-diol, 2,5-dimethyl-	142-30-3	0.0023	0.0008
140	3-Dodecanone	1534-27-6	0.019	0.004
25	3-Pentanol, 2-methyl-	565-67-3	0.00066	0.00059
135	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl	40702-26-9	0.0050	0.0003

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
36	3-Buten-2-one, 3-methyl-	814-78-8	0.0014	0.0002
149	4-Dodecanone, 11-methyl	29366-35-6	0.0084	0.0146
53	4-Heptanone	123-19-3	0.00022	0.00039
162	4-Tetradecanone	26496-20-8	0.013	0.0003
121	4-Nonene, 5-butyl- and others		0.0017	0.0003
161	4-Decanone	624-16-8	0.013	0.001
87	5-Undecene	4941-53-1	0.0010	0.0001
130	5-Decanone	820-29-1	0.00098	0.00005
79	5-Decene (E)	7433-56-9	0.0011	0.0001
125	6-Tridecene	24949-38-0	0.0012	0.0003
148	6-Tridecanone	22026-12-6	0.019	0.001
136	6-Dodecanone	6064-27-3	0.023	0.005
122	7-Tetradecene, (Z)-	41446-60-0	0.0025	0.0002
52	Acetamide, N-methyl-	79-16-3	0.00040	0.00070
23	Acetic acid	64-19-7	0.00061	0.00106
63	Acetonitrile, hydroxy-	107-16-4	0.00096	0.00166
91	Acetophenone	98-86-2	0.0028	0.00003
159	Alkyl cyclohexane		0.00092	0.00025
95	Benzene, nitro-	98-95-3	0.0037	0.0002
111	Benzene, 1-methyl-3-nitro-	99-08-1	0.0012	0.0001
177	Benzenesulfonamide, N-butyl	3622-84-2	0.0023	0.0023
101	Benzoic acid, 2-[(trimethylsilyl)oxy]-trimethyl	3789-85-3	0.00028	0.00048
19	Chloroform	67-66-3	0.0045	0.0007
44	cis-1-nitro-1-propene	27675-36-1	0.0080	0.0006
113	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.0010	0.00003
115	Cyclohexane, hexyl	4292-75-5	0.0019	0.0001
129	Cyclohexanol, 4-methyl-1-(1-methylethyl)-	470-65-5	0.00018	0.00032
151	Cyclohexanol, 4-methyl-1-(1-methylethyl)-	470-65-5	0.0011	0.0010

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
85	Cyclohexanone, 2,2,6-trimethyl	2408-37-9	0.00035	0.00031
150	Cyclohexene, 1-methyl-3-(1-methylethyl)-	13828-31-4	0.0018	0.0031
83	Cyclopentane, 1-ethyl-3-methyl-	2613-66-3	0.00039	0.00034
11	Cyclopropane, ethyl	1191-96-4	0.00042	0.00072
77	Cyclotetrasiloxane, octamethyl	556-67-2	0.0013	0.0013
48	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0023	0.0011
142	Decanamide, N-(2-hydroxyethyl)-	7726-08-1	0.0036	0.0032
80	Decane, 4-methyl-	2847-72-5	0.00071	0.000003
167	Diethyl Phthalate	84-66-2	0.00061	0.00053
143	Dodecanamide, N-(2-hydroxyethyl)-	142-78-9	0.0026	0.0045
116	Dodecane, 4-methyl-	6117-97-1	0.00087	0.00001
12	Ethane, 1,1,2-trichloro-1,2,2-trifluoro-	76-13-1	0.11	0.01
24	Ethane, 1,1,1-trichloro	71-55-6	0.00067	0.00058
7	Ethanol	64-17-5	0.026	0.003
3	Ethylene Oxide	75-21-8	0.017	0.030
21	Furan, tetrahydro-	109-99-9	0.0029	0.0008
120	Furan, tetrahydro-2, 5-dipropyl-	4457-62-9	0.0020	0.0003
138	Furan, tetrahydro-2, 5-dipropyl-	4457-62-9	0.0048	0.0011
62	Heptanal	111-71-7	0.0088	0.0005
103	Heptane, 3-ethyl-2-methyl-	14676-29-0	0.0014	0.0006
146	Hexadecane	544-76-3	0.0034	0.0002
179	Hexadecane, 7,9-dimethyl-	21164-95-4	0.00071	0.00020
46	Hexanal	66-25-1	0.0092	0.0006
82	Hexane, 2,5-dimethyl-	592-13-2	0.0021	0.0002
5	Hydrazine, 1,1-dimethyl	57-14-7	0.0031	0.0006
10	Isopropyl Alcohol	67-63-0	0.0071	0.0011
32	Isopropyl Alcohol	67-63-0	0.0010	0.0009
176	Isopropyl Myristate	110-27-0	0.00043	0.00075

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
185	Isopropyl Palmitate	142-91-6	0.00067	0.00065
6	Methane, dichlorofluoro-	75-43-4	0.0017	0.0002
2	Methyl alcohol and others		0.036	0.032
13	Methyl nitrate	598-58-3	0.031	0.002
102	n-Amylcyclohexane	4292-92-6	0.0011	0.0002
132	n-Amylcyclohexane	4292-92-6	0.00072	0.00124
20	Nitric acid, ethyl ester	625-58-1	0.031	0.002
30	Nitric acid, 1-methylethyl ester	1712-64-7	0.0046	0.0002
35	Nitric acid, propyl ester	627-13-4	0.027	0.001
49	Nitric acid, butyl ester	928-45-0	0.011	0.0003
55	Nitric acid, propyl ester and ethylbenzene		0.0014	0.0003
67	Nitric acid, pentyl ester	1002-16-0	0.0054	0.0003
81	Nitric acid, hexyl ester	20633-11-8	0.0040	0.0003
84	Nitric acid, pentyl ester	1002-16-0	0.00031	0.00054
99	Nitric acid, hexyl ester	20633-11-8	0.0029	0.0004
112	Nitric acid, nonyl ester	20633-13-0	0.0014	0.0003
114	Nonadecane, 9-methyl-	13287-24-6	0.00019	0.00032
96	Nonanal	124-19-6	0.0056	0.0008
98	Nonane, 3-methyl-5-propyl-	31081-18-2	0.00092	0.00015
133	Nonane, 4,5-dimethyl-	17302-23-7	0.0016	0.00001
78	Octanal	124-13-0	0.0068	0.0007
92	Octanenitrile	124-12-9	0.0024	0.0001
57	p-Xylene	106-42-3	0.00046	0.00043
153	Pentadecane	629-62-9	0.013	0.003
169	Pentadecane	629-62-9	0.00022	0.00038
31	Pentanal	110-62-3	0.011	0.001
15	Pentane, 2-methyl-	107-83-5	0.0012	0.0001
66	Pentanol, 5-amino	2508-29-4	0.0020	0.0017

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
38	Propane, 2-methyl-2-nitro-	594-70-7	0.0060	0.0002
58	Propane, 2-[(1,1-dimethylethyl) sulfonyl]-2-methyl-	1886-75-5	0.0023	0.0007
68	Propane, 2-ethoxy-2-methyl-	637-92-3	0.00036	0.00062
26	Propanenitrile, 2,2-dimethyl	630-18-2	0.0022	0.0013
37	Pyrazine	290-37-9	0.0025	0.0002
50	Pyridine, 3-methyl-	108-99-6	0.0023	0.0004
64	Pyridine, 2-ethyl-	100-71-0	0.00022	0.00039
127	Pyridine, 2,3,6-trimethyl	1462-84-6	0.00043	0.00037
9	Silane, chlorotrimethyl	75-77-4	0.00095	0.00165
186	Tetrachlorobiphenyl and others		0.00018	0.00031
47	Tetrachloroethylene	127-18-4	0.024	0.001
141	Tetradecane	629-59-4	0.30	0.01
65	trans-3,4-Dimethylcyclopentanone	19550-73-3	0.00021	0.00037
8	Trichlorofluoromethane	75-69-4	0.038	0.006
118	Tridecane, 7-methyl-	26730-14-3	0.0046	0.0001
145	Tridecane, 5-methyl-	25117-31-1	0.00070	0.00004
104	Undecane, 2-methyl-	7045-71-8	0.00075	0.00008
110	Undecane, 2,6-dimethyl-	17301-23-4	0.0025	0.0002
117	Undecane, 2,10-dimethyl-	17301-27-8	0.0015	0.0001
131	Undecane, 3-ethyl-	17312-58-2	0.0016	0.0014
123	Undecanenitrile	2244-07-7	0.0015	0.0013
Sum of tentatively identified compounds:			1.23	

1 CAS = Chemical Abstract Service.

2 Average of 3; 6-L TST samples, presented values are estimates.

Table 4-9
Tank TY-104 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)
141	Tetradecane	629-59-4	0.30	0.01
12	Ethane, 1,1,2-trichloro-1,2,2-trifluoro-	76-13-1	0.11	0.01
152	3-Tridecanone	1534-26-5	0.038	0.006
8	Trichlorofluoromethane	75-69-4	0.038	0.006
2	Methyl alcohol and others		0.036	0.032
20	Nitric acid, ethyl ester	625-58-1	0.031	0.002
13	Methyl nitrate	598-58-3	0.031	0.002
35	Nitric acid, propyl ester	627-13-4	0.027	0.001
16	1-Propanol	71-23-8	0.026	0.002
7	Ethanol	64-17-5	0.026	0.003
47	Tetrachloroethylene	127-18-4	0.024	0.001
136	6-Dodecanone	6064-27-3	0.023	0.005
148	6-Tridecanone	22026-12-6	0.019	0.001
140	3-Dodecanone	1534-27-6	0.019	0.004
18	2-Butanone	78-93-3	0.018	0.002
3	Ethylene Oxide	75-21-8	0.017	0.030
153	Pentadecane	629-62-9	0.013	0.003
161	4-Decanone	624-16-8	0.013	0.001
162	4-Tetradecanone	26496-20-8	0.013	0.0003
164	3-Tetradecanone	629-23-2	0.012	0.010
154	2-Tridecanone	593-08-8	0.011	0.003
49	Nitric acid, butyl ester	928-45-0	0.011	0.0003
31	Pentanal	110-62-3	0.011	0.001
46	Hexanal	66-25-1	0.0092	0.0006
62	Heptanal	111-71-7	0.0088	0.0005
149	4-Dodecanone, 11-methyl	29366-35-6	0.0084	0.0146

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
44	cis-1-nitro-1-propene	27675-36-1	0.0080	0.0006
10	Isopropyl Alcohol	67-63-0	0.0071	0.0011
139	2,2'-Bioxepane	74793-02-5	0.0069	0.0002
107	3-Dodecene, (E)-	7206-14-6	0.0069	0.0005
72	2-Heptanone, 6-methyl-	928-68-7	0.0068	0.0003
78	Octanal	124-13-0	0.0068	0.0007
59	3-Heptanone	106-35-4	0.0067	0.0003
38	Propane, 2-methyl-2-nitro-	594-70-7	0.0060	0.0002
165	2-Tetradecanone	2345-27-9	0.0057	0.0003
96	Nonanal	124-19-6	0.0056	0.0008
56	1-Hexanol	111-27-3	0.0055	0.0004
163	3-Dodecanone	1534-27-6	0.0055	0.0096
67	Nitric acid, pentyl ester	1002-16-0	0.0054	0.0003
76	1-Heptanol	111-70-6	0.0053	0.0005
135	3-Cyclohexene-1-carboxaldehyde, 1,3,4-trimethyl	40702-26-9	0.0050	0.0003
138	Furan, tetrahydro-2, 5-dipropyl-	4457-62-9	0.0048	0.0011
156	2-Decanol	1120-06-5	0.0048	0.0014
118	Tridecane, 7-methyl-	26730-14-3	0.0046	0.0001
30	Nitric acid, 1-methylethyl ester	1712-64-7	0.0046	0.0002
19	Chloroform	67-66-3	0.0045	0.0007
4	1-Propene, 2-methyl-	115-11-7	0.0042	0.0005
119	2(3H)-Furanone, 5-butyldihydro-	104-50-7	0.0041	0.0005
1	1-Propene, 2-methyl-	115-11-7	0.0040	0.0015
81	Nitric acid, hexyl ester	20633-11-8	0.0040	0.0003
178	1,1'-Biphenyl, 2,4',5-trichloro-	16606-02-3	0.0038	0.0009
95	Benzene, nitro-	98-95-3	0.0037	0.0002
86	1-Propanol, 2,2-dimethyl nitrate	926-42-1	0.0036	0.0004
142	Decanamide, N-(2-hydroxyethyl)-	7726-08-1	0.0036	0.0032

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
61	3-Heptanol	589-82-2	0.0036	0.0003
146	Hexadecane	544-76-3	0.0034	0.0002
105	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	0.0034	0.0005
108	2-Decanone	693-54-9	0.0032	0.0001
5	Hydrazine, 1,1-dimethyl	57-14-7	0.0031	0.0006
45	1-butanamine, N-ethylidene	6898-74-4	0.0030	0.0004
99	Nitric acid, hexyl ester	20633-11-8	0.0029	0.0004
90	1-Octanol	111-87-5	0.0029	0.0001
21	Furan, tetrahydro-	109-99-9	0.0029	0.0008
155	3-Dodecanol	10203-30-2	0.0028	0.0049
183	1,1'-Biphenyl, 2,3,3',5'-tetrachloro-	41464-49-7	0.0028	0.0002
91	Acetophenone	98-86-2	0.0028	0.00003
180	1,1'-Biphenyl, 2,4,4'-trichloro-	7012-37-5	0.0026	0.0006
143	Dodecanamide, N-(2-hydroxyethyl)-	142-78-9	0.0026	0.0045
122	7-Tetradecene, (Z)-	41446-60-0	0.0025	0.0002
37	Pyrazine	290-37-9	0.0025	0.0002
110	Undecane, 2,6-dimethyl-	17301-23-4	0.0025	0.0002
92	Octanenitrile	124-12-9	0.0024	0.0001
17	3-Buten-2-one	78-94-4	0.0024	0.0004
48	Cyclotrisiloxane, hexamethyl-	541-05-9	0.0023	0.0011
75	1-Hexene, 5,5-dimethyl-	7116-86-1	0.0023	0.0003
40	1-Pentanol	71-41-0	0.0023	0.0041
58	Propane, 2-[(1,1-dimethylethyl) sulfonyl]-2-methyl-	1886-75-5	0.0023	0.0007
50	Pyridine, 3-methyl-	108-99-6	0.0023	0.0004
160	1,1'-Biphenyl, 4-chloro	2051-62-9	0.0023	0.0001
177	Benzenesulfonamide, N-butyl	3622-84-2	0.0023	0.0023
147	3-Hexyne-2,5-diol, 2,5-dimethyl-	142-30-3	0.0023	0.0008
27	2-Butenal	4170-30-3	0.0022	0.0015

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
89	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.0022	0.0001
26	Propanenitrile, 2,2-dimethyl	630-18-2	0.0022	0.0013
94	2-Nonanone	821-55-6	0.0022	0.0002
82	Hexane, 2,5-dimethyl-	592-13-2	0.0021	0.0002
172	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.0020	0.0002
120	Furan, tetrahydro-2, 5-dipropyl-	4457-62-9	0.0020	0.0003
66	Pentanol, 5-amino	2508-29-4	0.0020	0.0017
115	Cyclohexane, hexyl	4292-75-5	0.0019	0.0001
106	1-Nonanol	143-08-8	0.0019	0.0004
42	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0019	0.0001
93	1-Decene, 5-methyl-	54244-79-0	0.0019	0.0001
150	Cyclohexene, 1-methyl-3-(1-methylethyl)-	13828-31-4	0.0018	0.0031
6	Methane, dichlorofluoro-	75-43-4	0.0017	0.0002
121	4-Nonene, 5-butyl- and others		0.0017	0.0003
133	Nonane, 4,5-dimethyl-	17302-23-7	0.0016	0.00001
34	1H-Imidazole, 2-methyl-	693-98-1	0.0016	0.0002
131	Undecane, 3-ethyl-	17312-58-2	0.0016	0.0014
28	2-Butanone, 3-methyl	563-80-4	0.0015	0.0017
137	2(3H)-Furanone, 5-heptyldihydro- and others		0.0057	0.0015
117	Undecane, 2,10-dimethyl-	17301-27-8	0.0015	0.0001
123	Undecanenitrile	2244-07-7	0.0015	0.0013
103	Heptane, 3-ethyl-2-methyl-	14676-29-0	0.0014	0.0006
173	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.0014	0.0002
112	Nitric acid, nonyl ester	20633-13-0	0.0014	0.0003
36	3-Buten-2-one, 3-methyl-	814-78-8	0.0014	0.0002
77	Cyclotetrasiloxane, octamethyl	556-67-2	0.0013	0.0013
109	1-Decene	872-05-9	0.0013	0.0001
54	2-Hexenal, (E)-	6728-26-3	0.0013	0.0005

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
22	1-Propanol, 2-methyl-	78-83-1	0.0013	0.0001
74	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	0.0013	0.0001
125	6-Tridecene	24949-38-0	0.0012	0.0003
157	2-Undecanol	1653-30-1	0.0012	0.0020
111	Benzene, 1-methyl-3-nitro-	99-08-1	0.0012	0.0001
15	Pentane, 2-methyl-	107-83-5	0.0012	0.0001
168	1,1'-Biphenyl, 2,2'-dichloro-	13029-08-8	0.0012	0.0001
102	n-Amylcyclohexane	4292-92-6	0.0011	0.0002
79	5-Decene (E)	7433-56-9	0.0011	0.0001
174	1,1'-Biphenyl, 2,3-dichloro-	16605-91-7	0.0011	0.0003
151	Cyclohexanol, 4-methyl-1-(1-methylethyl)-	470-65-5	0.0011	0.0010
87	5-Undecene	4941-53-1	0.0010	0.0001
32	Isopropyl Alcohol	67-63-0	0.0010	0.0009
70	2-Pentene, 2,4-dimethyl-	625-65-0	0.0010	0.0002
113	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.0010	0.00003
144	1-Methylcycloheptanol	3761-94-2	0.0010	0.0008
181	1,1'-Biphenyl, 2,3,4-trichloro-	55702-46-0	0.00091	0.00030
182	1,1'-Biphenyl, 2,3,4-trichloro-	55702-46-0	0.00094	0.00012
9	Silane, chlorotrimethyl	75-77-4	0.00095	0.00165
130	5-Decanone	820-29-1	0.00098	0.00005
159	Alkyl cyclohexane		0.00092	0.00025
73	3-Tetradecene, (E)-	41446-68-8	0.00093	0.00010
63	Acetonitrile, hydroxy-	107-16-4	0.00096	0.00166
88	1-Decanol, 2-ethyl	21078-65-9	0.00095	0.00009
171	1,1'-Biphenyl, 2,5-dichloro-	34883-39-1	0.00099	0.00006
98	Nonane, 3-methyl-5-propyl-	31081-18-2	0.00092	0.00015
29	1,4-Butanediamine	110-60-1	0.00080	0.00076
71	2-Pentanol, 2,3-dimethyl-	4911-70-0	0.00087	0.00011

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
116	Dodecane, 4-methyl-	6117-97-1	0.00087	0.00001
179	Hexadecane, 7,9-dimethyl-	21164-95-4	0.00071	0.00020
39	3-Pentanone, 2-methyl-	565-69-5	0.00076	0.00018
80	Decane, 4-methyl-	2847-72-5	0.00071	0.000003
104	Undecane, 2-methyl-	7045-71-8	0.00075	0.00008
132	n-Amylcyclohexane	4292-92-6	0.00072	0.00124
145	Tridecane, 5-methyl-	25117-31-1	0.00070	0.00004
43	3-Hexanone	589-38-8	0.00070	0.00003
97	2-Undecene, (Z)-	821-96-5	0.00060	0.00008
24	Ethane, 1,1,1-trichloro	71-55-6	0.00067	0.00058
23	Acetic acid	64-19-7	0.00061	0.00106
25	3-Pentanol, 2-methyl-	565-67-3	0.00066	0.00059
185	Isopropyl Palmitate	142-91-6	0.00067	0.00065
175	1,1'-Biphenyl, 4,4'-dichloro-	2050-68-2	0.00066	0.00114
167	Diethyl Phthalate	84-66-2	0.00061	0.00053
158	(S)-1-Amino-2-(methoxymethyl)-pyrrolidine	59983-39-0	0.00060	0.00104
14	2-Propen-1-ol	107-18-6	0.00059	0.00051
124	2-Pyrrolidinone	616-45-5	0.00053	0.00091
127	Pyridine, 2,3,6-trimethyl	1462-84-6	0.00043	0.00037
57	p-Xylene	106-42-3	0.00046	0.00043
100	2-Hexanone, 6-methoxy-	29006-00-6	0.00044	0.00039
134	1-Pyrrolidinecarboxaldehyde	3760-54-1	0.00040	0.00035
60	2-Nonene, (E)-	6434-78-2	0.00043	0.00039
11	Cyclopropane, ethyl	1191-96-4	0.00042	0.00072
33	2-Heptene, (E)-	14686-13-6	0.00046	0.00080
176	Isopropyl Myristate	110-27-0	0.00043	0.00075
52	Acetamide, N-methyl-	79-16-3	0.00040	0.00070
166	1,1'-Biphenyl, 4-chloro	2051-62-9	0.00049	0.00044

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Nitric acid, propyl ester and ethylbenzene		0.0014	0.0003
84	Nitric acid, pentyl ester	1002-16-0	0.00031	0.00054
85	Cyclohexanone, 2,2,6-trimethyl	2408-37-9	0.00035	0.00031
41	2-Pentanone, 3-methyl-	565-61-7	0.00037	0.00032
68	Propane, 2-ethoxy-2-methyl-	637-92-3	0.00036	0.00062
83	Cyclopentane, 1-ethyl-3-methyl-	2613-66-3	0.00039	0.00034
69	2,3-Dimethyl-2-hexanol	19550-03-9	0.00022	0.00038
101	Benzoic acid, 2-[(trimethylsilyl)oxy]-trimethyl	3789-85-3	0.00028	0.00048
64	Pyridine, 2-ethyl-	100-71-0	0.00022	0.00039
65	trans-3,4-Dimethylcyclopentanone	19550-73-3	0.00021	0.00037
184	1,1'-Biphenyl, 2,3,4',6-tetrachloro-	52663-58-8	0.00020	0.00034
53	4-Heptanone	123-19-3	0.00022	0.00039
51	1-Hexene, 4,5-dimethyl-	16106-59-5	0.00020	0.00034
169	Pentadecane	629-62-9	0.00022	0.00038
126	1-Ethylpropyl octanoate and others		0.00023	0.00041
114	Nonadecane, 9-methyl-	13287-24-6	0.00019	0.00032
128	1-Methyl-2-(4-methylpentyl)-cyclopentane		0.00018	0.00032
129	Cyclohexanol, 4-methyl-1-(1-methylethyl)-	470-65-5	0.00018	0.00032
170	2-Heptadecanone	2922-51-2	0.00018	0.00031
186	Tetrachlorobiphenyl and others		0.00018	0.00031
Sum of tentatively identified compounds:			1.23	

1 CAS = Chemical Abstract Service.

2 Average of 3, 6-L TST samples, presented values are estimates.

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