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Accession #: D196054794

Document #: SD-WM-ER-447

Title/Desc:

TANK 241T107 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
1/1995

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COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN 626289

Proj. ECN

2. ECN Category (mark one) <input type="checkbox"/> Supplemental <input checked="" type="checkbox"/> Direct Revision <input type="checkbox"/> Change ECN <input type="checkbox"/> Temporary <input type="checkbox"/> Standby <input type="checkbox"/> Supersedeure <input type="checkbox"/> Cancel/Void	3. Originator's Name, Organization, MSIN, and Telephone No. D. R. BRATZEL, 75640, S7-21, 373-3579		3a. USQ Required? <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No	4. Date 09/27/95
	5. Project Title/No./Work Order No. TANK 241-T-107 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN JANUARY 1995		6. Bldg./Sys./Fac. No. 2704HV/200E	7. Approval Designator N/A
	8. Document Numbers Changed by this ECN (includes sheet no. and rev.) WHC-SD-WM-ER-447 REV 10		9. Related ECN No(s). N/A	10. Related PO No. N/A
11a. Modification Work <input type="checkbox"/> Yes (fill out Blk. 11b) <input checked="" type="checkbox"/> No (NA Blks. 11b, 11c, 11d)	11b. Work Package No. N/A	11c. Modification Work Complete N/A Cog. Engineer Signature & Date	11d. Restored to Original Condition (Temp. or Standby ECN only) N/A Cog. Engineer Signature & Date	

12. Description of Change
Title change and complete rewrite.

13a. Justification (mark one)

Criteria Change <input checked="" type="checkbox"/>	Design Improvement <input type="checkbox"/>	Environmental <input type="checkbox"/>	Facility Deactivation <input type="checkbox"/>
As-Found <input type="checkbox"/>	Facilitate Const <input type="checkbox"/>	Const. Error/Omission <input type="checkbox"/>	Design Error/Omission <input type="checkbox"/>

13b. Justification Details
Complete rewrite which includes all vapor sampling events to date and data qualification.

14. Distribution (include name, MSIN, and no. of copies)
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1. ECN (use no. from pg. 1)

626289

15. Design Verification Required <input type="checkbox"/> Yes <input checked="" type="checkbox"/> No	16. Cost Impact <table style="width: 100%; border: none;"> <tr> <td style="width: 50%; text-align: center;">ENGINEERING</td> <td style="width: 50%; text-align: center;">CONSTRUCTION</td> </tr> <tr> <td>Additional <input type="checkbox"/> \$</td> <td>Additional <input type="checkbox"/> \$</td> </tr> <tr> <td>Savings <input type="checkbox"/> \$</td> <td>Savings <input type="checkbox"/> \$</td> </tr> </table>	ENGINEERING	CONSTRUCTION	Additional <input type="checkbox"/> \$	Additional <input type="checkbox"/> \$	Savings <input type="checkbox"/> \$	Savings <input type="checkbox"/> \$	17. Schedule Impact (days) Improvement <input type="checkbox"/> Delay <input type="checkbox"/>
ENGINEERING	CONSTRUCTION							
Additional <input type="checkbox"/> \$	Additional <input type="checkbox"/> \$							
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18. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 12. Enter the affected document number in Block 19.

SDD/DD	<input type="checkbox"/>	Seismic/Stress Analysis	<input type="checkbox"/>	Tank Calibration Manual	<input type="checkbox"/>
Functional Design Criteria	<input type="checkbox"/>	Stress/Design Report	<input type="checkbox"/>	Health Physics Procedure	<input type="checkbox"/>
Operating Specification	<input type="checkbox"/>	Interface Control Drawing	<input type="checkbox"/>	Spares Multiple Unit Listing	<input type="checkbox"/>
Criticality Specification	<input type="checkbox"/>	Calibration Procedure	<input type="checkbox"/>	Test Procedures/Specification	<input type="checkbox"/>
Conceptual Design Report	<input type="checkbox"/>	Installation Procedure	<input type="checkbox"/>	Component Index	<input type="checkbox"/>
Equipment Spec.	<input type="checkbox"/>	Maintenance Procedure	<input type="checkbox"/>	ASME Coded Item	<input type="checkbox"/>
Const. Spec.	<input type="checkbox"/>	Engineering Procedure	<input type="checkbox"/>	Human Factor Consideration	<input type="checkbox"/>
Procurement Spec.	<input type="checkbox"/>	Operating Instruction	<input type="checkbox"/>	Computer Software	<input type="checkbox"/>
Vendor Information	<input type="checkbox"/>	Operating Procedure	<input type="checkbox"/>	Electric Circuit Schedule	<input type="checkbox"/>
OM Manual	<input type="checkbox"/>	Operational Safety Requirement	<input type="checkbox"/>	ICRS Procedure	<input type="checkbox"/>
FSAR/SAR	<input type="checkbox"/>	IEFD Drawing	<input type="checkbox"/>	Process Control Manual/Plan	<input type="checkbox"/>
Safety Equipment List	<input type="checkbox"/>	Cell Arrangement Drawing	<input type="checkbox"/>	Process Flow Chart	<input type="checkbox"/>
Radiation Work Permit	<input type="checkbox"/>	Essential Material Specification	<input type="checkbox"/>	Purchase Requisition	<input type="checkbox"/>
Environmental Impact Statement	<input type="checkbox"/>	Fac. Proc. Samp. Schedule	<input type="checkbox"/>	Tickler File	<input type="checkbox"/>
Environmental Report	<input type="checkbox"/>	Inspection Plan	<input type="checkbox"/>		<input type="checkbox"/>
Environmental Permit	<input type="checkbox"/>	Inventory Adjustment Request	<input type="checkbox"/>		<input type="checkbox"/>

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.

Document Number/Revision	Document Number/Revision	Document Number Revision

20. Approvals

	Signature	Date		Signature	Date
<u>OPERATIONS AND ENGINEERING</u>			<u>ARCHITECT-ENGINEER</u>		
Cog. Eng. D. R. Bratzel	<i>DR Bratzel</i>	9/25/95	PE		
Cog. Mgr. T. J. Kelley	<i>TJ Kelley</i>	9/25/95	QA		
QA			Safety		
Safety			Design		
Environ.			Environ.		
Other			Other		
Proj.					
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			<u>ADDITIONAL</u>		

SEP 27 1995

RELEASE AUTHORIZATION

Document Number: WHC-SD-WM-ER-447, REV 1

Document Title: Tank 241-T-107 Headspace Gas and Vapor
Characterization Results for Samples Collected in
January 1995

Release Date: 9/26/95

**This document was reviewed following the
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WHC Information Release Administration Specialist:


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SUPPORTING DOCUMENT1. Total Pages *40*

2. Title

TANK 241-T-107 HEADSPACE GAS AND VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
JANUARY 1995

3. Number

WHC-SD-WM-ER-447

4. Rev No.

1

5. Key Words

CHARACTERIZATION OBJECTIVES, TANK HEADSPACE,
SAMPLING EVENT, INORGANIC GASES, ORGANIC VAPORS

6. Author

Name: D. R. BRATZEL


Signature *DR Bratzel 9/25/95*

Organization/Charge Code 75640/N4AB1

7. Abstract

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

8. RELEASE STAMP

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RECORD OF REVISION		(1) Document Number	Page 1	
(2) Title TANK 241-T-107 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN JANUARY 1995				
CHANGE CONTROL RECORD				
(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release		
		(5) Cog. Engr.	(6) Cog. Mgr.	Date
0	(7) WHC-SD-WM-ER-447, REV. 0, EDT 612339 May 31, 1995			
RS 1	Complete revision and title change. ECN 626289	<i>DRB</i>	<i>Kelly</i>	<i>2/2/95</i>

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Tank 241-T-107 Headspace Gas and Vapor Characterization Results for Samples Collected in January 1995

J. L. Huckaby
Pacific Northwest Laboratories

D. R. Bratzel
Westinghouse Hanford Company

Date Published
September 1995

Prepared for the U.S. Department of Energy
Office of Environmental Restoration and
Waste Management



Westinghouse P.O. Box 1970
Hanford Company Richland, Washington

Management and Operations Contractor for the
U.S. Department of Energy under Contract DE-AC06-87RL10930

Approved for Public Release

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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

Acknowledgements

The authors wish to thank Chris Simonen for her work verifying data and generating tables, and Shas Mattigod for his help with the construction and reviews of this document. The authors also wish to thank Luther Buckley, Clarence Homi, and Tom Kunthara for their contributions to the final reviews and publication of this document.

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**Tank 241-T-107 Headspace Gas and Vapor Characterization Results
for Samples Collected in January 1995**

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank T-107 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank T-107 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994). Results presented here represent the best available data on the headspace constituents of tank T-107.

1.2 Characterization Data Criteria

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

Single Shell Tank Interim Operational Safety Requirements (Dougherty 1995) specifies that combustible constituents in tank headspaces be maintained below 25 % of the lower flammability limit (LFL). This essentially agrees with National Fire Protection Association requirements that combustible concentrations be maintained at or below 25 % of the LFL (NFPA 1992). Current governing operating specifications for Watchlist tanks, such as tank T-107, 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 T-107 headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been representative of the tank headspace when the tank was sampled (Meacham et al. 1995), and sample analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment has been made of how the tank T-107 headspace composition changes with time, though studies of tank C-103 suggest that composition changes probably occur very slowly in passively ventilated tanks, such as tank T-107 (Huckaby and Story 1994).

1.4 Tank Headspace Dynamics

Tank T-107 is the first tank in a 3-tank cascade with tanks T-108 and T-109. It is connected to tank T-108 via a 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade line. A similar cascade line connects tanks T-108 and T-109. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank T-108 or tank T-109 may be transferred to tank T-107 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for either tanks T-108 or T-109 to assess their potential effect on tank T-107.

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

2.0 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank T-107 using the vapor sampling system (VSS) on January 18, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-T-107 Tank Characterization Plan* (Homi 1995a). Air from the tank T-107 headspace was withdrawn from a single elevation 5.5 m below the riser flange via a heated vapor sampling probe/instrument tree mounted in riser 5, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. All tank air samples were collected between 5:00 p.m. and 9:00 p.m., with no anomalies noted.

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

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

3.0 INORGANIC GASES AND VAPORS

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

Analyses of inorganic analytes in sorbent traps and SUMMATM canisters were performed within 29 and 35 days, respectively, after sample collection (Ligotke 1995). This was within the allowed 60-day holding time of the WHC quality assurance project plan (Keller 1994). It should be noted that the 60-day holding time was administratively chosen, and that analytical holding times have not been established by an appropriate study of analyte stabilities in the sampling devices and in the chemical matrix of the tank air samples.

3.1 Ammonia, Hydrogen, and Nitrous Oxide

Ammonia concentration in the headspace of tank T-107 was measured to be 125 ppmv. Ammonia has been observed in virtually all of the 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 125 ppmv corresponds to about 0.08 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank T-107 was measured to be < 94 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, the < 94 ppmv hydrogen detection limit corresponds to about < 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank T-107.

The nitrous oxide concentration in tank T-107 was measured to be 41.5 ppmv. Nitrous oxide has been detected in other waste tanks at concentrations as low as about 12 ppmv in tank TX-105 (KJinger et al. 1995), and as high as about 868 ppmv in tank U-103 (Ligotke et al. 1995). Under the 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 T-107 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank T-107 headspace was determined to be < 12 ppmv. In ambient air carbon monoxide 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. 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

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

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 T-107 headspace, measured to be an average 75 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 T-107 gas and vapor sampling event, for example, were measured to have an average 365 ppmv of carbon dioxide (Pool et al. 1995a).

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank T-107 headspace were determined to be ≤ 0.05 ppmv and ≤ 0.03 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank T-107. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. These constituents could potentially serve as oxidizers to support combustion, but at the measured concentrations would have a negligible effect on the flammability of the tank T-107 headspace.

The water vapor concentration of tank T-107 was determined to be about 12.1 mg/L, for a headspace temperature of 17.2 °C and the measured headspace pressure of 989 mbar (742.8 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 16.2 mbar (12.1 torr), to a dew point of 14.2 °C, and to a relative humidity of 82 %. This relative humidity is similar to that of other tanks that hold primarily sludge.

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

3.4 Discussion of Inorganic Gases and Vapors

Aside from water and carbon dioxide, the most abundant waste constituents in the tank T-107 headspace are ammonia and nitrous oxide. Along with hydrogen, they have been detected in most tank headspaces sampled to date, and are usually the dominate waste species.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good. Relative standard deviations range from about 1.3 % for water vapor to 15 % for nitrous oxide. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), the small

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.

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 T-107 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatographs (GCs) equipped with mass spectrometer (MS) detectors were used by both laboratories to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Pool et al. (1995).

PNL SUMMA™ sample results should be considered to be the primary organic vapor data for tank T-107. All PNL sample preparation and analyses were performed at PNL quality assurance impact level 2. Analyses of SUMMA™ canisters for organic vapors by PNL was completed within 49 days of sample collection (Ligothke 1995). It should be noted that though this satisfied the administratively chosen 60-day holding time (Keller 1994), no holding time study has been performed to address the stability of organic compounds in SUMMA™ canisters in the likely chemical matrix of the waste tanks.

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.

ORNL analyzed 4 of the 12 TST tank samples, 1 of the 2 TST field blanks, and 1 of the 2 TST trip blanks. ORNL analyzed a single 4-L TST tank sample to estimate the concentration of organic vapors sampled. Because the measured organic vapor concentrations were higher than optimum for 4-L samples, the 1-L TST tank samples were analyzed for analyte identification and quantification.

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 both means and standard deviations within the 95 % confidence interval for variance, indicating that no bias was introduced in the measurement of analyte quantities.

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 from analysis of known compounds. 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 was comprised of the 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method list, which consists primarily of halocarbons and common industrial solvents, plus 14 analytes selected from the toxicology panel's review of tank C-103.

Propanone (acetone), ethanenitrile (acetonitrile), and 2-butanone were the only SUMMA™ sample target analytes detected above the 0.005 ppmv quantitation limit. The average concentrations of these compounds in the 3 SUMMA™ samples is given in Table 4-1. Analysis was performed according to the TO-14 methodology by PNL (EPA 1988, Pool et al. 1995).

Jenkins et al. (1995a) report the positive identification of 24 of 27 target analytes in TST samples. 1,1-Dichloroethene, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected in the TST samples. The average concentrations of the target analytes, from the analysis of 3 TSTs, are given in Tables 4-2, 4-3, and 4-4. Target analytes for which all of the measured concentrations were within the calibration range of the instrument, and for which analyses were within their practical holding times, are listed in Table 4-2. Target analytes for which 1 or more of the measured concentrations were outside the calibration range are listed in Table 4-3. The 3 target analytes for which the ORNL practical holding times were exceeded are listed in Table 4-4. Tables 4-2, 4-3, and 4-4 are mutually exclusive, so that no analyte appears in more than 1 of these tables. Data in Tables 4-3 and 4-4 should not be considered quantitative and may not be accurate to within $\pm 30\%$ as specified by Burnum (1995).

The ORNL practical holding time is defined as the holding time for which there is a 15% risk that the concentration of an analyte in the sample will be below its initial concentration. As indicated in Table 4-4, butanal, 1-butanol, and 2-pentanone, exceeded their practical holding times, and may have been affected by the 44 day period between sample collection and analysis (Jenkins 1995). Jenkins et al. (1995b) describe the ORNL practical holding time study, and report the practical holding times of butanal, 1-butanol, and 2-pentanone are 1, 17, and 34 days, respectively. It should be noted 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. The results given may be corrected for the measured water vapor content of tank T-107 to obtain concentration in ppmv of analyte in moist tank air by multiplying the dry-air ppmv concentrations by 0.985.

Table 4-5 lists the 11 target analytes were common to both TST and SUMMA™ analyses, and their reported average concentrations in TST and SUMMA™ samples. The reported TST sample concentrations of chlorinated compounds (i.e., 1,1-dichloroethene and dichloromethane) and nonpolar compounds (i.e., benzene, toluene, n-hexane, n-heptane, and n-decane) in Table 4-5 are all ≤ 0.0012 ppmv, and well below the SUMMA™ analysis method detection limit of 0.005 ppmv.

The propanone (acetone) concentration in the SUMMA™ samples was reported to be over 7 times as high as in TST samples. There is a similar disagreement regarding the ethanenitrile (acetonitrile) concentration in SUMMA™ and TST samples from tank T-107. As shown in Table 4-5, the average concentration of ethanenitrile in SUMMA™ samples was more than 3 times that in TST samples. In lieu of reasons to discount either results, the higher values should be used as the best measurement of such compounds.

4.2 Tentatively Identified Organic Compounds

In addition to the target analytes, the ORNL and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and may also determine its molecular weight. The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Using this method, many analytes can be tentatively identified with reasonable

confidence without having to inject each into the GC/MS to determine their GC retention times or specific MS patterns.

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and 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 list of tentatively identified compounds recovered from SUMMA™ samples and their estimated concentrations, is given in Table 4-6. Compounds are listed in Table 4-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples and their estimated concentrations, is given in Table 4-7. Compounds are listed in Table 4-7 according to the order by which they eluted chromatographically. The averages reported by ORNL in Table 4-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

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

Concentrations given in Tables 4-6 through 4-7 should be considered rough estimates. Also, results in Tables 4-6 through 4-7 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks or the assignment of the same identity to different peaks (e.g., Cmpd # 53 and 62 in Table 4-7). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995a) and Pool et al. (1995), respectively, and should be reviewed before this data are used for decision making. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

4.3 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables 4-1 through 4-9 is to separate them into 2 categories: 1) organic compounds added to tank T-107 as waste that are still evaporating, and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes the tentatively identified alkyl-substituted decahydronaphthalenes, and semivolatile branched and straight-chain alkanes. These were used as diluents of tributyl phosphate in various plutonium extraction processes. The semivolatile straight-chain alkanes (i.e., n-undecane, n-dodecane, n-tridecane, n-

tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs).

The tentatively identified cyclosiloxanes and silanes (i.e., Cmpd # 3, 11, 37, and 55 in Table 4-7) are also in this category. Small quantities of siloxanes may have been introduced to the waste tank through disposal of hydraulic fluids, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables 4-1 through 4-9 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, alkyl nitrates, and volatile alkanes, all of which have been associated with the degradation of the NPHs. The hydrolysis of tributyl phosphate, for example, is thought to be the principal source of 1-butanol. By far the most abundant of these in the headspace are the short-chain volatile compounds, however, near the bottom of Table 4-7 are several long-chain low volatility compounds that are also probably waste reaction products.

Samples from tank T-107 were found to have a several alkyl nitrates (i.e., nitric acid esters). Though it is reasonable to expect alkyl nitrates to be produced via chemical and radiolytic processes of the NPHs with other waste, their solubility in the aqueous waste supernates would also be expected to significantly reduce their vapor-phase concentrations. That these constituents are at detectible levels in tank T-107 may indicate dry conditions where they are formed.

The notable absence of tributyl phosphate in the tank T-107 samples may be due to a sampling difficulty. The presence of the tributyl phosphate diluents and their degradation products is reason to expect tributyl phosphate to be present in the tank waste. 1-Butanol, which was the fourth most abundant compound found in 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 concentration of tributyl phosphate in the tank T-107 headspace should be considered to be unknown.

Though there are many compounds listed in Tables 4-1 through 4-9, the tank T-107 headspace has a relatively low total organic vapor concentration. The sum of quantitatively measured and estimated TST organic analyte concentrations, by GC/MS analyses, is 1.4 mg/m³ (Jenkins et al. 1995a).

In summary, the organic vapor concentrations in tank T-107 are relatively low. While not completely typical of NPH-rich tanks, the organic vapors in tank T-107 clearly indicate the presence of trace amounts of the semivolatile NPHs and their degradation products. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

5.0 SUMMARY

The tank T-107 headspace was sampled in January 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 1995b).

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Table 2-1
 Tank T-107 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.2	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
		3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank
		3.0	Nitric Oxide	6 tank air samples + 3 trip blank
WHC 222-S Laboratory	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
		6.0	Organic vapors	3 tank air samples + 2 ambient air samples
		1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
Tank T-107 Inorganic Gas and Vapor Concentrations --
Analyses Conducted by Pacific Northwest Laboratory

Compound	CAS ¹ number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Ammonia, NH ₃	7664-41-7	Sorbent Trap	6	125	2	6
Carbon dioxide, CO ₂	124-38-9	SUMMA™	3	75	10	13
Carbon monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 94	--	--
Nitric oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.05	--	10
Nitrogen dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.03	--	--
Nitrous oxide, N ₂ O	10024-97-2	SUMMA™	3	41.5	6.2	15
Water vapor, H ₂ O	7732-18-5	Sorbent Trap	6	16,300 (12.1 mg/L)	200 (0.2 mg/L)	1.3

1 CAS = Chemical Abstracts Service.

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

Table 4-1
Tank T-107 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	Propanone (acetone)	67-64-1	0.93	0.062	7
2	2-Butanone	78-93-3	0.033	0.005	15
3	Ethanenitrile (acetonitrile)	75-05-8	0.17	0.008	5
4	Methane	74-82-8	< 61	--	--

1 CAS = Chemical Abstract Service.

2 Average of 3 samples.

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

Table 4-2
Tank T-107 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	0.048	0.018	37
2	n-Tridecane	629-50-5	0.0056	0.0019	33

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

2 CAS = Chemical Abstract Service.

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

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

Table 4-3
Tank T-107 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	0.12	0.05	46
2	Dichloromethane (methylene chloride)	75-09-2	0.00061	0.00063	104
3	Propanenitrile	107-12-0	0.0031	0.0024	77
4	n-Hexane	110-54-3	0.00078	0.00030	38
5	Benzene	71-43-2	0.00076	0.00031	41
6	n-Butanenitrile	109-74-0	0.0054	0.0012	22
7	n-Heptane	142-82-5	0.00049	0.00018	37
8	Toluene	108-88-3	0.0012	0.0004	33
9	n-Pentanenitrile	110-59-8	0.0018	0.0003	17
10	2-Hexanone	591-78-6	0.00073	0.00016	21
11	n-Octane	111-65-9	0.00042	0.00010	23
12	n-Hexanenitrile	628-73-9	0.0011	0.0002	16
13	2-Heptanone	110-43-0	0.00074	0.00020	27
14	n-Nonane	111-84-2	0.00028	0.00013	47
15	n-Heptanenitrile	629-08-3	0.00079	0.00009	12
16	2-Octanone	111-13-7	0.00033	0.00007	20
17	n-Decane	124-18-5	0.00052	0.00010	19
18	n-Undecane	1120-21-4	0.0015	0.0002	11
19	n-Dodecane	112-70-3	0.0021	0.0004	21

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 4-L and 1 was 1-L.

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

Table 4-4
Tank T-107 Positively Identified Organic Compounds in TST Samples
for which Practical Holding Times were Exceeded --
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	Butanal ⁵	123-72-8	0.00027	0.00055	200
2	1-Butanol ⁶	71-36-3	0.023	0.0036	16
3	2-Pentanone ⁵	107-87-9	0.0030	0.0008	27

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 4-L and 1 was 1-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.

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

Table 4-5
Tank T-107 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Oak Ridge National Laboratory
and Pacific Northwest Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	RPD ⁴ (%)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.00058	< 0.005	--
Dichloromethane (methylene chloride)	75-09-2	0.00061	< 0.005	--
Propanone (acetone)	67-64-1	0.12	0.93	154
Ethananitrile (acetonitrile)	75-05-8	0.048	0.17	112
Propanenitrile	107-12-0	0.0031	< 0.005	--
n-Butanenitrile	109-74-0	0.0054	< 0.005	> 8
Benzene	71-43-2	0.00076	< 0.005	--
Toluene	108-88-3	0.0012	< 0.005	--
n-Hexane	110-54-3	0.00078	< 0.005	--
n-Heptane	142-82-5	0.00049	< 0.005	--
n-Decane	124-18-5	0.00052	< 0.005	--

1 CAS = Chemical Abstract Service.

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

3 Average of 3 samples.

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

Table 4-6
Tank T-107 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 ⁴	74-98-6	0.22	0.005
2	Methanol (methyl alcohol)	67-56-1	1.11	0.07
3	Ethanol ⁵	64-17-5	0.12	--
4	1-Butanol	71-36-3	0.09	< 0.005
Sum of tentatively identified compounds:			1.92	

1 CAS = Chemical Abstract Service.

2 Average of 3 samples. Values given are estimates.

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

4 Detected in only 2 samples.

5 Detected in only 1 sample.

Table 4-7
Tank T-107 Tentatively Identified Organic Compounds in TST Samples
in Order of Chromatographic Elution --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Methyl Alcohol	67-56-1	0.13	0.01
2	Methyl formate	107-31-3	0.00075	0.00130
3	Silane, fluorotrimethyl-	420-56-4	0.00066	0.00114
4	Methane, dichlorofluoro-	75-43-4	0.00076	0.00132
5	Ethanol	64-17-5	0.023	0.004
6	Trichloromonofluoromethane	75-69-4	0.038	0.054
7	Isopropyl Alcohol	67-63-0	0.020	0.006
8	Nitric acid, methyl ester	598-58-3	0.00078	0.00136
9	Pentane, 2-methyl-	107-83-5	0.0013	0.0012
10	1-Propanol	71-23-8	0.010	0.002
11	Silanol, trimethyl-	1066-40-6	0.0026	0.0005
12	2-Butanone	78-93-3	0.0024	0.0023
13	1-Hexene, 3,4-dimethyl-	16745-94-1	0.00063	0.00109
14	Nitric acid, ethyl ester	625-58-1	0.0053	0.0034
15	1-Propanol, 2-methyl-	78-83-1	0.00066	0.00115
16	Furan, tetrahydro-	109-99-9	0.00053	0.00092
17	Acetic acid, methyl ester	79-20-9	0.028	0.016
18	Acetic acid	64-19-7	0.024	0.021
19	2-Butanone, 3-methyl-	563-80-4	0.00072	0.00125
20	3-Pentanone	96-22-0	0.0032	0.0006
21	2-Butanol	78-92-2	0.0038	0.0010
22	2-Butanone, 3,3-dimethyl-	75-97-8	0.0020	0.0004
23	Nitric acid, propyl ester	627-13-4	0.0071	0.0007
24	Propanoic acid	79-09-4	0.0012	0.0011
25	2-Pentanol, 2-methyl-	590-36-3	0.00052	0.00090
26	Pyrazine	290-37-9	0.0034	0.0017

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
27	Butane, 1-nitro-	627-05-4	0.0018	0.0016
28	2-Hexanol, 5-methyl-	627-59-8	0.0028	0.0007
29	3-Pentanone, 2-methyl-	565-69-5	0.00051	0.00089
30	2-Pentene, 2-methoxy-	61142-47-0	0.0016	0.0014
31	2-Pentanone, 3-methyl-	565-61-7	0.00047	0.00081
32	Propylene Glycol	57-55-6	0.023	0.024
33	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0023	0.0002
34	3-Hexanone	589-38-8	0.0017	0.0002
35	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.011	0.001
36	Tetrachloroethylene	127-18-4	0.010	0.002
37	Cyclotrisiloxane, hexamethyl-	541-05-9	0.014	0.006
38	Nitric acid, butyl ester	928-45-0	0.0070	0.0006
39	1-Hexanol and others		0.0020	0.0003
40	Cycloheptane, 1,3-dimethoxy-, trans-	29887-79-4	0.0021	0.0003
41	Ethylbenzene and others		0.00046	0.00079
42	1-Hexanol	111-27-3	0.0071	0.0011
43	p-Xylene	106-42-3	0.0010	0.0009
44	1-Pentene, 4,4-dimethyl-	762-62-9	0.0025	0.0004
45	3-Heptanone	106-35-4	0.0044	0.0003
46	2-Heptanol	543-49-7	0.0021	0.0004
47	Heptanal	111-71-7	0.0030	0.0005
48	3-Aminopropionitrile	151-18-8	0.0024	0.0001
49	Nitric acid, pentyl ester	1002-16-0	0.0036	0.0006
50	3-Ethyl-2-methyl-2-pentanol		0.00042	0.00073
51	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.00046	0.00080
52	2-Heptanone, 6-methyl-	928-68-7	0.0072	0.0008
53	1-Hexanol, 2-ethyl-	104-76-7	0.0050	0.0002
54	1-Heptanol	111-70-6	0.0072	0.0005

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
55	Cyclotetrasiloxane, octamethyl-	556-67-2	0.010	0.009
56	.alpha.-Methylstyrene and others		0.0012	0.0011
57	Benzonitrile	100-47-0	0.0020	0.0003
58	Octanal	124-13-0	0.0028	0.0004
59	Cyclopropane, 1-ethyl-2-pentyl-	62238-08-8	0.0016	0.0002
60	Nonane, 2,6-dimethyl-	17302-28-2	0.0020	0.00002
61	Nitric acid, hexyl ester	20633-11-8	0.0015	0.0001
62	1-Hexanol, 2-ethyl-	104-76-7	0.017	0.005
63	Mixture		0.0011	0.0010
64	Benzyl Alcohol	100-51-6	0.0012	0.0010
65	Cyclohexanone, 3,3,5-trimethyl-	873-94-9	0.0016	0.0001
66	5-Undecene	4941-53-1	0.0023	0.0002
67	Decane , 2-methyl-	6975-98-0	0.0005	0.0009
68	1-Octanol	111-87-5	0.0025	0.0001
69	Decahydronaphthalene	493-02-7	0.00048	0.00083
70	Phenol, 3-methyl-	108-39-4	0.0019	0.0001
71	Acetophenone	98-86-2	0.0041	0.0009
72	Octanenitrile	124-12-9	0.0048	0.0003
73	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.0028	0.0003
74	2-Nonanone	821-55-6	0.0020	0.0001
75	Nonanal	124-19-6	0.0087	0.0001
76	Naphthalene, decahydro-2-methyl- and others		0.0020	0.0017
77	Benzoic acid, 2-[(trimethylsilyloxy) trimethyl]	3789-85-3	0.0040	0.0006
78	Cyclohexane, pentyl-	4292-92-6	0.0016	0.0002
79	Hexane, 2,3,3-trimethyl-	16747-28-7	0.0021	0.0010
80	Nonanol	28473-21-4	0.0032	0.0011
81	Nonanenitrile	2243-27-8	0.0026	0.0022

WHC-SD-WM-ER-447 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
82	2-Decanone	693-54-9	0.0024	0.00005
83	Ethanone, 1-(3-methylphenyl)-	585-74-0	0.0012	0.0010
84	Decanal	112-31-2	0.0034	0.0001
85	Undecane, 2,6-dimethyl-	17301-23-4	0.0024	0.0003
86	Benzene, 1-methyl-4-nitro-	99-99-0	0.0020	0.0003
87	Benzene, 1-methyl-4-nitro- & cyclohexane, 2-butyl-1,1, 3-trimethyl-		0.0016	0.0001
88	Cyclohexane, hexyl-	4292-75-5	0.0022	0.0005
89	Benothiazole	95-16-9	0.0038	0.0003
90	Decane, 2-methyl-	6975-98-0	0.0046	0.0005
91	2(3H)-Furanone, 5-ethylidihydro-	695-06-7	0.0020	0.0001
92	4-Undecanol	4272-06-4	0.0024	0.0006
93	1-Octadecyne	629-89-0	0.0019	0.0002
94	Tridecane, 6-methyl-	13287-21-3	0.0013	0.0011
95	Tridecane, 4-methyl-	26730-12-1	0.0021	0.0004
96	Tridecane, 2-methyl-	1560-96-9	0.0015	0.0013
97	Undecane, 2,9-dimethyl-	17301-26-7	0.0014	0.0012
98	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.016	0.003
99	Butanoic acid, 1-methylpropyl ester	819-97-6	0.00046	0.00080
100	Tetradecane	629-59-4	0.030	0.007
101	Decane, 2,3,5-trimethyl-	62238-11-3	0.0025	0.0008
102	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.0011	0.0010
103	Diphenyl ether	101-84-8	0.0024	0.0002
104	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.00092	0.00159
105	Tetradecane, 5-methyl-	25117-32-2	0.00058	0.00100
106	Tetradecane, 4-methyl-	25117-24-2	0.0014	0.0012
107	Decane, 5-propyl-	17312-62-8	0.028	0.007
108	Tetradecane, 3-methyl-	18435-22-8	0.0029	0.0008
109	6-Dodecanone	6064-27-3	0.0016	0.0002

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
110	Tetradecane	629-59-4	0.0016	0.0001
111	2,5-Cyclohexadiene-1,4-dione, 2,6-bis-(1,1-dimethylethyl)-	719-22-2	0.00058	0.00101
112	Pentadecane	629-62-9	0.040	0.012
113	Cyclohexane, 1,(1,5-dimethylhexyl)-	29799-19-7	0.0014	0.0012
114	Nonane, 2-methyl-5-propyl-	31081-17-1	0.00072	0.00125
115	Hexadecane, 7,9-dimethyl-	21164-95-4	0.0020	0.0018
116	Undecane, 4-methyl-	2980-69-0	0.00045	0.00078
117	Octadecane, 2-methyl-	1560-88-9	0.0020	0.0017
118	Cyclohexane, (4-methylpentyl)-	61142-20-9	0.0026	0.0006
119	Tridecane, 2-methyl-	1560-96-9	0.00046	0.00079
120	Tetradecane, 6,9-dimethyl-	55045-13-1	0.00045	0.00078
121	Hexadecane	544-76-3	0.016	0.006
122	2-Furanmethanol, tetrahydro-, acetate	637-64-9	0.0030	0.0003
123	Octanal, 7-hydroxy-3,7-dimethyl	107-75-5	0.00044	0.00076
124	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.0036	0.0012
125	Heptadecane	629-78-7	0.0033	0.0009
126	Octadecane, 2,6-dimethyl-	75163-97-2	0.0012	0.0010
127	Benzenesulfonamide, N-butyl-	3622-84-2	0.021	0.002
128	Octadecane	593-45-3	0.017	0.018
129	Isopropyl Palmitate	142-91-6	0.0037	0.0020
Sum of tentatively identified compounds:			0.78	

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 4-L and 1 was 1-L. Values given are estimates.

Table 4-8
Tank T-107 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
56	.alpha.-Methylstyrene and others		0.0012	0.0011
15	1-Propanol, 2-methyl-	78-83-1	0.00066	0.00115
62	1-Hexanol, 2-ethyl-	104-76-7	0.017	0.005
54	1-Heptanol	111-70-6	0.0072	0.0005
13	1-Hexene, 3,4-dimethyl-	16745-94-1	0.00063	0.00109
42	1-Hexanol	111-27-3	0.0071	0.0011
44	1-Pentene, 4,4-dimethyl-	762-62-9	0.0025	0.0004
68	1-Octanol	111-87-5	0.0025	0.0001
53	1-Hexanol, 2-ethyl-	104-76-7	0.0050	0.0002
39	1-Hexanol and others		0.0020	0.0003
93	1-Octadecyne	629-89-0	0.0019	0.0002
10	1-Propanol	71-23-8	0.010	0.002
12	2-Butanone	78-93-3	0.0024	0.0023
28	2-Hexanol, 5-methyl-	627-59-8	0.0028	0.0007
52	2-Heptanone, 6-methyl-	928-68-7	0.0072	0.0008
46	2-Heptanol	543-49-7	0.0021	0.0004
25	2-Pentanol, 2-methyl-	590-36-3	0.00052	0.00090
74	2-Nonanone	821-55-6	0.0020	0.0001
122	2-Furanmethanol, tetrahydro-, acetate	637-64-9	0.0030	0.0003
30	2-Pentene, 2-methoxy-	61142-47-0	0.0016	0.0014
31	2-Pentanone, 3-methyl-	565-61-7	0.00047	0.00081
19	2-Butanone, 3-methyl-	563-80-4	0.00072	0.00125
33	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0023	0.0002
82	2-Decanone	693-54-9	0.0024	0.00005
21	2-Butanol	78-92-2	0.0038	0.0010
22	2-Butanone, 3,3-dimethyl-	75-97-8	0.0020	0.0004

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
91	2(3H)-Furanone, 5-ethylidihydro-	695-06-7	0.0020	0.0001
111	2,5-Cyclohexadiene-1,4-dione, 2,6-bis-(1,1-dimethylethyl)-	719-22-2	0.00058	0.00101
35	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.011	0.001
29	3-Pentanone, 2-methyl-	565-69-5	0.00051	0.00089
20	3-Pentanone	96-22-0	0.0032	0.0006
34	3-Hexanone	589-38-8	0.0017	0.0002
50	3-Ethyl-2-methyl-2-pentanol		0.00042	0.00073
48	3-Aminopropionitrile	151-18-8	0.0024	0.0001
45	3-Heptanone	106-35-4	0.0044	0.0003
92	4-Undecanol	4272-06-4	0.0024	0.0006
66	5-Undecene	4941-53-1	0.0023	0.0002
109	6-Dodecanone	6064-27-3	0.0016	0.0002
18	Acetic acid	64-19-7	0.024	0.021
17	Acetic acid, methyl ester	79-20-9	0.028	0.016
71	Acetophenone	98-86-2	0.0041	0.0009
87	Benzene, 1-methyl-4-nitro- & cyclohexane, 2-butyl-1,1, 3-trimethyl-		0.0016	0.0001
86	Benzene, 1-methyl-4-nitro-	99-99-0	0.0020	0.0003
127	Benzenesulfonamide, N-butyl-	3622-84-2	0.021	0.002
77	Benzoic acid, 2-[(trimethylsilyloxy) trimethyl]	3789-85-3	0.0040	0.0006
57	Benzonitrile	100-47-0	0.0020	0.0003
89	Benzothiazole	95-16-9	0.0038	0.0003
64	Benzyl Alcohol	100-51-6	0.0012	0.0010
27	Butane, 1-nitro	627-05-4	0.0018	0.0016
99	Butanoic acid, 1-methylpropyl- ester	819-97-6	0.00046	0.00080
40	Cycloheptane, 1,3-dimethoxy-, trans	29887-79-4	0.0021	0.0003
113	Cyclohexane, 1,(1,5-dimethylhexyl)-	29799-19-7	0.0014	0.0012

WHC-SD-WM-ER-447 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
51	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.00046	0.00080
88	Cyclohexane, hexyl-	4292-75-5	0.0022	0.0005
118	Cyclohexane, (4-methylpentyl)-	61142-20-9	0.0026	0.0006
78	Cyclohexane, pentyl-	4292-92-6	0.0016	0.0002
73	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.0028	0.0003
65	Cyclohexanone, 3,3,5-trimethyl-	873-94-9	0.0016	0.0001
59	Cyclopropane, 1-ethyl-2-pentyl-	62238-08-8	0.0016	0.0002
55	Cyclotetrasiloxane, octamethyl-	556-67-2	0.010	0.009
37	Cyclotrisiloxane, hexamethyl-	541-05-9	0.014	0.006
69	Decahydronaphthalene	493-02-7	0.00048	0.00083
84	Decanal	112-31-2	0.0034	0.0001
90	Decane, 2-methyl-	6975-98-0	0.0046	0.0005
67	Decane, 2-methyl-	6975-98-0	0.0005	0.0009
101	Decane, 2,3,5-trimethyl-	62238-11-3	0.0025	0.0008
107	Decane, 5-propyl-	17312-62-8	0.028	0.007
103	Diphenyl ether	101-84-8	0.0024	0.0002
98	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.016	0.003
104	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.00092	0.00159
5	Ethanol	64-17-5	0.023	0.004
83	Ethanone, 1-(3-methylphenyl)-	585-74-0	0.0012	0.0010
41	Ethylbenzene and others		0.00046	0.00079
16	Furan, tetrahydro-	109-99-9	0.00053	0.00092
125	Heptadecane	629-78-7	0.0033	0.0009
47	Heptanal	111-71-7	0.0030	0.0005
121	Hexadecane	544-76-3	0.016	0.006
124	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.0036	0.0012
115	Hexadecane, 7,9-dimethyl-	21164-95-4	0.0020	0.0018
79	Hexane, 2,3,3-trimethyl-	16747-28-7	0.0021	0.0010

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
129	Isopropyl Palmitate	142-91-6	0.0037	0.0020
7	Isopropyl Alcohol	67-63-0	0.020	0.006
4	Methane, dichlorofluoro-	75-43-4	0.00076	0.00132
2	Methyl formate	107-31-3	0.00075	0.00130
1	Methyl Alcohol	67-56-1	0.13	0.01
63	Mixture		0.0011	0.0010
76	Naphthalene, decahydro-2-methyl- and others		0.0020	0.0017
61	Nitric acid, hexyl ester	20633-11-8	0.0015	0.0001
49	Nitric acid, pentyl ester	1002-16-0	0.0036	0.0006
14	Nitric acid, ethyl ester	625-58-1	0.0053	0.0034
23	Nitric acid, propyl ester	627-13-4	0.0071	0.0007
8	Nitric acid, methyl ester	598-58-3	0.00078	0.00136
38	Nitric acid, butyl ester	928-45-0	0.0070	0.0006
75	Nonanal	124-19-6	0.0087	0.0001
114	Nonane, 2-methyl-5-propyl-	31081-17-1	0.00072	0.00125
102	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.0011	0.0010
60	Nonane, 2,6-dimethyl-	17302-28-2	0.0020	0.00002
81	Nonanenitrile	2243-27-8	0.0026	0.0022
80	Nonanol	28473-21-4	0.0032	0.0011
126	Octadecane, 2,6-dimethyl-	75163-97-2	0.0012	0.0010
128	Octadecane	593-45-3	0.017	0.018
117	Octadecane, 2-methyl-	1560-88-9	0.0020	0.0017
123	Octanal, 7-hydroxy-3,7-dimethyl-	107-75-5	0.00044	0.00076
58	Octanal	124-13-0	0.0028	0.0004
72	Octanenitrile	124-12-9	0.0048	0.0003
43	p-Xylene	106-42-3	0.0010	0.0009
112	Pentadecane	629-62-9	0.040	0.012
9	Pentane, 2-methyl-	107-83-5	0.0013	0.0012

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
70	Phenol, 3-methyl-	108-39-4	0.0019	0.0001
24	Propanoic acid	79-09-4	0.0012	0.0011
32	Propylene Glycol	57-55-6	0.023	0.024
26	Pyrazine	290-37-9	0.0034	0.0017
3	Silane, fluorotrimethyl-	420-56-4	0.00066	0.00114
11	Silanol, trimethyl-	1066-40-6	0.0026	0.0005
36	Tetrachloroethylene	127-18-4	0.010	0.002
106	Tetradecane, 4-methyl-	25117-24-2	0.0014	0.0012
100	Tetradecane	629-59-4	0.030	0.007
120	Tetradecane, 6,9-dimethyl-	55045-13-1	0.00045	0.00078
108	Tetradecane, 3-methyl-	18435-22-8	0.0029	0.0008
105	Tetradecane, 5-methyl-	25117-32-2	0.00058	0.00100
110	Tetradecane	629-59-4	0.0016	0.0001
6	Trichloromonofluoromethane	75-69-4	0.038	0.054
96	Tridecane, 2-methyl-	1560-96-9	0.0015	0.0013
95	Tridecane, 4-methyl-	26730-12-1	0.0021	0.0004
94	Tridecane, 6-methyl-	13287-21-3	0.0013	0.0011
119	Tridecane, 2-methyl-	1560-96-9	0.00046	0.00079
85	Undecane, 2,6-dimethyl-	17301-23-4	0.0024	0.0003
116	Undecane, 4-methyl-	2980-69-0	0.00045	0.00078
97	Undecane, 2,9-dimethyl-	17301-26-7	0.0014	0.0012

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 4-L and 1 was 1-L. Values given are estimates.

Table 4-9
Tank T-107 Tentatively Identified Organic Compounds in TST Samples
Sorted by Estimated Concentration --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Methyl Alcohol	67-56-1	0.13	0.01
112	Pentadecane	629-62-9	0.040	0.012
6	Trichloromonofluoromethane	75-69-4	0.038	0.054
100	Tetradecane	629-59-4	0.030	0.007
17	Acetic acid, methyl ester	79-20-9	0.028	0.016
107	Decane, 5-propyl-	17312-62-8	0.028	0.007
18	Acetic acid	64-19-7	0.024	0.021
32	Propylene Glycol	57-55-6	0.023	0.024
5	Ethanol	64-17-5	0.023	0.004
127	Benzenesulfonamide, N-butyl-	3622-84-2	0.021	0.002
7	Isopropyl Alcohol	67-63-0	0.020	0.006
128	Octadecane	593-45-3	0.017	0.018
62	1-Hexanol, 2-ethyl-	104-76-7	0.017	0.005
121	Hexadecane	544-76-3	0.016	0.006
98	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.016	0.003
37	Cyclotrisiloxane, hexamethyl-	541-05-9	0.014	0.006
35	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.011	0.001
36	Tetrachloroethylene	127-18-4	0.010	0.002
55	Cyclotetrasiloxane, octamethyl-	556-67-2	0.010	0.009
10	1-Propanol	71-23-8	0.010	0.002
75	Nonanal	124-19-6	0.0087	0.0001
54	1-Heptanol	111-70-6	0.0072	0.0005
52	2-Heptanone, 6-methyl-	928-68-7	0.0072	0.0008
42	1-Hexanol	111-27-3	0.0071	0.0011
23	Nitric acid, propyl ester	627-13-4	0.0071	0.0007
38	Nitric acid, butyl ester	928-45-0	0.0070	0.0006

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Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
14	Nitric acid, ethyl ester	625-58-1	0.0053	0.0034
53	1-Hexanol, 2-ethyl-	104-76-7	0.0050	0.0002
72	Octanenitrile	124-12-9	0.0048	0.0003
90	Decane, 2-methyl-	6975-98-0	0.0046	0.0005
45	3-Heptanone	106-35-4	0.0044	0.0003
71	Acetophenone	98-86-2	0.0041	0.0009
77	Benzoic acid, 2-[(trimethylsilyloxy) trimethyl]	3789-85-3	0.0040	0.0006
21	2-Butanol	78-92-2	0.0038	0.0010
89	Benzothiazole	95-16-9	0.0038	0.0003
129	Isopropyl Palmitate	142-91-6	0.0037	0.0020
49	Nitric acid, pentyl ester	1002-16-0	0.0036	0.0006
124	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	0.0036	0.0012
26	Pyrazine	290-37-9	0.0034	0.0017
84	Decanal	112-31-2	0.0034	0.0001
125	Heptadecane	629-78-7	0.0033	0.0009
80	Nonanol	28473-21-4	0.0032	0.0011
20	3-Pentanone	96-22-0	0.0032	0.0006
122	2-Furanmethanol, tetrahydro-, acetate	637-64-9	0.0030	0.0003
47	Heptanal	111-71-7	0.0030	0.0005
108	Tetradecane, 3-methyl-	18435-22-8	0.0029	0.0008
73	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.0028	0.0003
58	Octanal	124-13-0	0.0028	0.0004
28	2-Hexanol, 5-methyl-	627-59-8	0.0028	0.0007
81	Nonanenitrile	2243-27-8	0.0026	0.0022
11	Silanol, trimethyl-	1066-40-6	0.0026	0.0005
118	Cyclohexane, (4-methylpentyl)-	61142-20-9	0.0026	0.0006
44	1-Pentene, 4,4-dimethyl-	762-62-9	0.0025	0.0004
101	Decane, 2,3,5-trimethyl-	62238-11-3	0.0025	0.0008

WHC-SD-WM-ER-447 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
68	1-Octanol	111-87-5	0.0025	0.0001
12	2-Butanone	78-93-3	0.0024	0.0023
85	Undecane, 2,6-dimethyl-	17301-23-4	0.0024	0.0003
103	Diphenyl ether	101-84-8	0.0024	0.0002
92	4-Undecanol	4272-06-4	0.0024	0.0006
82	2-Decanone	693-54-9	0.0024	0.00005
48	3-Aminopropionitrile	151-18-8	0.0024	0.0001
33	2-Pentanone, 4,4-dimethyl-	590-50-1	0.0023	0.0002
66	5-Undecene	4941-53-1	0.0023	0.0002
88	Cyclohexane, hexyl-	4292-75-5	0.0022	0.0005
95	Tridecane, 4-methyl-	26730-12-1	0.0021	0.0004
46	2-Heptanol	543-49-7	0.0021	0.0004
40	Cycloheptane, 1,3-dimethoxy-, trans	29887-79-4	0.0021	0.0003
79	Hexane, 2,3,3-trimethyl-	16747-28-7	0.0021	0.0010
60	Nonane, 2,6-dimethyl-	17302-28-2	0.0020	0.00002
76	Naphthalene, decahydro-2-methyl- and others		0.0020	0.0017
22	2-Butanone, 3,3-dimethyl-	75-97-8	0.0020	0.0004
91	2(3H)-Furanone, 5-ethylidihydro-	695-06-7	0.0020	0.0001
117	Octadecane, 2-methyl-	1560-88-9	0.0020	0.0017
74	2-Nonanone	821-55-6	0.0020	0.0001
57	Benzonitrile	100-47-0	0.0020	0.0003
86	Benzene, 1-methyl-4-nitro-	99-99-0	0.0020	0.0003
115	Hexadecane, 7,9-dimethyl-	21164-95-4	0.0020	0.0018
39	1-Hexanol and others		0.0020	0.0003
93	1-Octadecyne	629-89-0	0.0019	0.0002
70	Phenol, 3-methyl-	108-39-4	0.0019	0.0001
27	Butane, 1-nitro-	627-05-4	0.0018	0.0016
34	3-Hexanone	589-38-8	0.0017	0.0002

WHC-SD-WM-ER-447 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
87	Benzene, 1-methyl-4-nitro- & cyclohexane, 2-butyl-1,1, 3-trimethyl-		0.0016	0.0001
110	Tetradecane	629-59-4	0.0016	0.0001
30	2-Pentene, 2-methoxy-	61142-47-0	0.0016	0.0014
65	Cyclohexanone, 3,3,5-trimethyl-	873-94-9	0.0016	0.0001
78	Cyclohexane, pentyl-	4292-92-6	0.0016	0.0002
109	6-Dodecanone	6064-27-3	0.0016	0.0002
59	Cyclopropane, 1-ethyl-2-pentyl-	62238-08-8	0.0016	0.0002
96	Tridecane, 2-methyl-	1560-96-9	0.0015	0.0013
61	Nitric acid, hexyl ester	20633-11-8	0.0015	0.0001
97	Undecane, 2,9-dimethyl-	17301-26-7	0.0014	0.0012
106	Tetradecane, 4-methyl-	25117-24-2	0.0014	0.0012
113	Cyclohexane, 1,(1,5-dimethylhexyl)-	29799-19-7	0.0014	0.0012
9	Pentane, 2-methyl-	107-83-5	0.0013	0.0012
94	Tridecane, 6-methyl-	13287-21-3	0.0013	0.0011
24	Propanoic acid	79-09-4	0.0012	0.0011
83	Ethanone, 1-(3-methylphenyl)-	585-74-0	0.0012	0.0010
126	Octadecane, 2,6-dimethyl-	75163-97-2	0.0012	0.0010
56	.alpha.-Methylstyrene and others		0.0012	0.0011
64	Benzyl Alcohol	100-51-6	0.0012	0.0010
102	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.0011	0.0010
63	Mixture		0.0011	0.0010
43	p-Xylene	106-42-3	0.0010	0.0009
104	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.00092	0.00159
8	Nitric acid, methyl ester	598-58-3	0.00078	0.00136
19	2-Butanone, 3-methyl-	563-80-4	0.00072	0.00125
114	Nonane, 2-methyl-5-propyl-	31081-17-1	0.00072	0.00125
4	Methane, dichlorofluoro-	75-43-4	0.00076	0.00132
2	Methyl formate	107-31-3	0.00075	0.00130

WHC-SD-WM-ER-447 REV. 1

Cmpd #	Compound	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
13	1-Hexene, 3,4-dimethyl-	16745-94-1	0.00063	0.00109
3	Silane, fluorotrimethyl-	420-56-4	0.00066	0.00114
15	1-Propanol, 2-methyl-	78-83-1	0.00066	0.00115
16	Furan, tetrahydro-	109-99-9	0.00053	0.00092
105	Tetradecane, 5-methyl-	25117-32-2	0.00058	0.00100
111	2,5-Cyclohexadiene-1,4-dione, 2,6-bis-(1,1-dimethylethyl)-	719-22-2	0.00058	0.00101
29	3-Pentanone, 2-methyl-	565-69-5	0.00051	0.00089
25	2-Pentanol, 2-methyl-	590-36-3	0.00052	0.00090
67	Decane, 2-methyl-	6975-98-0	0.0005	0.0009
41	Ethylbenzene and others		0.00046	0.00079
50	3-Ethyl-2-methyl-2-pentanol		0.00042	0.00073
51	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.00046	0.00080
99	Butanoic acid, 1-methylpropyl ester	819-97-6	0.00046	0.00080
31	2-Pentanone, 3-methyl-	565-61-7	0.00047	0.00081
69	Decahydronaphthalene	493-02-7	0.00048	0.00083
116	Undecane, 4-methyl-	2980-69-0	0.00045	0.00078
123	Octanal, 7-hydroxy-3,7-dimethyl-	107-75-5	0.00044	0.00076
120	Tetradecane, 6,9-dimethyl-	55045-13-1	0.00045	0.00078
119	Tridecane, 2-methyl-	1560-96-9	0.00046	0.00079

1 CAS = Chemical Abstract Service.

2 Average of 4 TST samples: 3 were 4-L and 1 was 1-L. Values given are estimates.

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