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Accession #: D196054914

Document #: SD-WM-ER-506

Title/Desc:

TANK 241AX102 HEADSPACE GAS & VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
6/1995

SEP 28 1995

ENGINEERING DATA TRANSMITTAL

Page 1 of 1
1. EDT No 613577

2. To: (Receiving Organization) DISTRIBUTION		3. From: (Originating Organization) TWRS/CHARACTERIZATION PROJECT		4. Related EDT No.: N/A	
5. Proj./Prog./Dept./Div.: TWRS/CHAR PROJECT		6. Cog. Engr.: D. R. BRATZEL		7. Purchase Order No.: N/A	
8. Originator Remarks: N/A				9. Equip./Component No.: N/A	
				10. System/Bldg./Facility: 2704HV/200E	
11. Receiver Remarks:				12. Major Assm. Dwg. No.: N/A	
				13. Permit/Permit Application No.: N/A	
				14. Required Response Date: 09/27/95	

15. DATA TRANSMITTED					(F)	(G)	(H)	(I)
(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	Approval Designator	Reason for Transmittal	Originator Disposition	Receiver Disposition
1	WHC-SD-WM-ER-506		0	TANK 241-AX-102 HEADSPACE GAS AND VAPOR CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN JUNE 1995	<i>DR</i> <i>N/A</i> <i>THD</i> <i>9/27/95</i>	1	1	

16. KEY					
Approval Designator (F)		Reason for Transmittal (G)		Disposition (H) & (I)	
E, S, Q, D or N/A (see WHC-CM-3-5, Sec.12.7)		1. Approval 2. Release 3. Information	4. Review 5. Post-Review 6. Dist. (Receipt Acknow. Required)	1. Approved 2. Approved w/comment 3. Disapproved w/comment	4. Reviewed no/comment 5. Reviewed w/comment 6. Receipt acknowledged

(G)	(H)	17. SIGNATURE/DISTRIBUTION (See Approval Designator for required signatures)								(G)	(H)
Reason	Disp.	(J) Name	(K) Signature	(L) Date	(M) MSIN	(J) Name	(K) Signature	(L) Date	(M) MSIN	Reason	Disp.
1	1	Cog. Eng. D. R. BRATZEL	<i>DRB</i>	<i>9/25/95</i>							
1	1	Cog. Mgr. T. J. KELLEY	<i>TJK</i>	<i>9/25/95</i>							
		QA									
		Safety									
		Env.									

18. D. R. BRATZEL <i>DRB</i> Signature of EDT Originator		19. N/A Authorized Representative Date for Receiving Organization		20. <i>TJK</i> Cognizant Manager Date		21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments	
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RELEASE AUTHORIZATION

Document Number: WHC-SD-WM-ER-506, REV 0

Document Title: Tank 241-AX-102 Headspace Gas and Vapor
Characterization Results for Samples Collected in
June 1995

Release Date: 9/28/95

**This document was reviewed following the
procedures described in WHC-CM-3-4 and is:**

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SUPPORTING DOCUMENT1. Total Pages *46*

2. Title

TANK 241-AX-102 HEADSPACE GAS AND VAPOR
CHARACTERIZATION RESULTS FOR SAMPLES COLLECTED IN
JUNE 1995

3. Number

WHC-SD-WM-ER-506

4. Rev No.

0

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.

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Tank 241-AX-102 Headspace Gas and Vapor Characterization Results for Samples Collected in June 1995

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Date Published
September 1995

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

Westinghouse
Hanford Company

P.O. Box 1970
Richland, Washington

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

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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%
TO-14	task order 14
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-AX-102 Headspace Gas and Vapor Characterization Results
for Samples Collected in June 1995

1.0 INTRODUCTION

1.1 Characterization Objectives

Tank AX-102 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 AX-102 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1995).

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 1994). However, current governing operating specifications for Watchlist waste tanks, such as tank AX-102 specify that combustible constituents be maintained at or below 20 % of the LFL (WHC 1995a).

Headspace characterization data is 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. 1995).

1.3 Sampling Overview

Tank headspace characterization data presented here are from a single sampling event. Samples collected are thought to have been representative of tank AX-102 headspace when the tank was sampled (Meacham et al. 1995), and samples analyses were designed to provide a reasonably accurate and complete characterization of the significant headspace constituents. No assessment has been made as to how the tank AX-102 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 AX-102 is the second tank in a 3-tank cascade with tanks AX-101 and AX-103. It is connected to each of these tanks via 7.4-cm (2.9-in.) inside diameter, 7.6-m (25-ft) long underground cascade lines. Since these cascade lines connect the headspaces of these tanks, gases and vapors originating from the wastes in tank AX-101 or tank AX-103 may be transferred to tank AX-102 (unless the cascade lines are obstructed). At this time, however, no headspace characterization data are available for tank AX-101 or AX-103 to assess their potential transfer of gases and vapors to tank AX-102.

The cascade of tanks AX-101, AX-102, and AX-103 is passively ventilated, which means that the tanks are allowed to exhale air, waste gases, and vapors as the barometric pressure falls, and inhale ambient air as the barometric pressure rises. Each of these tanks has its own filtered breather riser. Barometric pressure typically rises and falls on a diurnal cycle, producing an average daily exchange of air equal to about 0.46 % of each tank headspace (Huckaby 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 AX-102 using the vapor sampling system (VSS) on June 27, 1995 by WHC Sampling and Mobile Laboratories (WHC 1995b). Sample collection and analysis were performed as directed by *Tank 241-AX-102 Tank Characterization Plan* (Homi 1995a). The tank headspace temperature was determined to be 24.6 °C. Air from the AX-102 headspace was withdrawn from a single elevation via a 7.9-m long heated sampling probe mounted in riser 9E, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 60 °C. All tank air samples were collected between 10:46 a.m. and 12:59 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 52 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 16 trip blanks and 16 field blanks provided by the laboratories.

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

3.0 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA^{TM,1} canister tank air samples for selected inorganic gases and vapors are given in Table 3-1 in parts per million by volume (ppmv) in dry air. The concentration of water vapor 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 (Clauss et al. 1995).

Analyses of inorganic analytes in sorbent traps and SUMMATM canisters were performed within 24 and 3 days, respectively, after sample collection. 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

The concentration of ammonia in the headspace of tank AX-102 was determined to be 34 ppmv from 6 sorbent trap samples. 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 34 ppmv corresponds to about 0.02 % of the LFL, and does not contribute appreciably to the flammability of the headspace.

The concentration of hydrogen in tank AX-102 was determined to be < 98 ppmv in each of the 3 SUMMATM canister samples. Hydrogen in the waste tanks is of concern as a fuel. Given that the LFL for hydrogen in air is about 4 vol%, the < 98 ppmv hydrogen concentration in tank AX-102 corresponds to < 0.25 % of its LFL. At this level, hydrogen is not a flammability concern in tank AX-102.

The nitrous oxide concentration in tank AX-102 was determined to be 50 ppmv from 3 SUMMATM canister samples. Nitrous oxide has been detected in other passively ventilated waste tanks at average concentrations as low as about 12 ppmv in tank TX-105 (Klinger et al. 1995), and as high as 878 ppmv in tank U-103 (Ligotke et al. 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 AX-102 headspace.

3.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank AX-102 headspace was reported to be < 12 ppmv. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are

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

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 AX-102 headspace, measured to be 704 ppmv, is significantly higher than it is in ambient air. In most tanks that have been sampled the headspace carbon dioxide concentration is lower than it is in ambient air, though several exceptions are known. 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 between about 10 ppmv to 200 ppmv in the waste tank headspaces. The ambient air samples collected at the start of the tank AX-102 sampling event, for example, contained an average 332 ppmv of carbon dioxide.

The apparent explanation for higher than ambient levels of carbon dioxide in tank AX-102 is that the waste liquids in the tank have relatively high levels of carbonate. Sederberg (1995) examined a similar situation in tank C-101, where the headspace carbon dioxide concentration was measured to be an average [1,426 ppmv]³. Sederberg found that at the measured pH and waste temperature, the carbonate concentration of waste liquid in tank C-101 was high enough to evolve carbon dioxide (rather than absorb it). Several other tanks have since been observed to have higher than ambient carbon dioxide concentrations, including tanks C-107 and B-103.

3.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank AX-102 headspace were determined to be 0.18 and ≤ 0.08 ppmv, respectively. These are acid gases that would have very low equilibrium concentrations above the high pH sludge in tank AX-102. 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 AX-102 headspace.

The water vapor concentration of tank AX-102 was determined to be about 11.9 mg/L, at the measured tank headspace temperature of 24.6 °C and pressure of 996 mbar (747 torr), (WHC 1995b). This corresponds to a water vapor partial pressure of 16.4 mbar (12.3 torr), to a dew point of 14.4 °C, and to a relative humidity of 53 %.

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-

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

³ This value was determined by Oregon Graduate Institute of Science and Technology, and should be considered a secondary result (Burnum 1995). Huckaby and Bratzel (1995) provide further details and supporting data.

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 AX-102 headspace are carbon dioxide, ammonia, and nitrous oxide. Carbon dioxide is apparently desorbed by the waste, where it would exist as some form of carbonate in solution. The carbonate in tank AX-102 was probably introduced as a waste constituent, and is not being generated within the tank. Ammonia and nitrous oxide, by contrast, are thought to be produced by chemical and radiolytic reactions of the waste.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table 3-1 are good for the methods used. Relative standard deviations range from about 0.9 % for carbon dioxide, to about 9 % for ammonia. Because the precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

4.0 ORGANIC VAPORS

Organic vapors in the tank AX-102 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by both PNL and ORNL. To the extent possible, identical sets of TSTs were collected for PNL and ORNL, though each laboratory prepared their own samples. Both PNL and ORNL 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. (1995) and Clauss et al. (1995).

PNL SUMMA™ results should be considered the primary organic vapor data for tank AX-102. These results were produced at PNL quality assurance impact level 2. PNL preparation and analyses of TST samples were performed at PNL quality assurance impact level 3. PNL analyses of TSTs and SUMMA™ canisters for organic vapors were completed 30 and 8 days, respectively, after sample collection. These satisfied the administratively chosen 60-day holding time (Keller 1994). PNL has not conducted holding time studies to determine the stability of organic compounds in either SUMMA™ canisters or TSTs in the chemical matrix of the tank air samples.

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

All TSTs prepared by ORNL had 3 surrogate compounds added to evaluate sample matrix effects, potential handling, storage, and shipment problems, and analytical instrumentation performance. 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 et al. 1995).

PNL used the same number and type of surrogate spikes as were used by ORNL. Surrogate recoveries by PNL were comparable to those of ORNL, but the ORNL statistical criteria are not directly applicable. A statistical treatment of PNL surrogate recoveries, similar to that done by ORNL, has not been performed in part because of insufficient data. Surrogates have been used by PNL only as indicators of gross sample matrix, handling, storage, and shipment problems, and no such problems were indicated in the tank AX-102 TST samples.

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 the 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 from 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 tank C-103. For cost efficiencies, PNL analyzed for the same set of target analytes in both SUMMATM and TST samples. This was also done to obtain maximum comparison of the methods.

Table 4-1 lists the organic compounds positively identified and quantitated in SUMMATM samples. Results given in Table 4-1 were obtained using the EPA TO-14 methodology, except for analysis of methane, which was analyzed with the inorganic gases (Clauss et al. 1995). Only 9 organic analytes were positively identified in SUMMATM samples (1 from the TO-14 list of 39 analytes, and 8 from the list of additional analytes). Others were determined to be present below the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMATM canister samples. The precision of the SUMMATM sample measurements was good, as indicated by the very small relative standard deviations given in the last column of Table 4-1.

The positively identified and quantitated analytes in PNL TST samples, with their average concentrations, are listed in Table 4-2. These are also given with the analogous PNL SUMMATM canister results in Table 4-3 for comparison. In addition to the 9 analytes positively identified in SUMMATM canisters, 2 other analytes (dichloromethane and toluene) were also detected in the TST samples. These 2 additional analytes were determined to be virtually at the detection limit of the analyses. In general, the agreement between these 2 methods is quite good, as indicated by the calculated relative percent differences in the last column of Table 4-3. As with the SUMMATM sample analyses, target analytes not reported in Table 4-2 were deemed to be below the 0.005 ppmv detection limit. The largest discrepancy between the 2 methods is for the measurement of 1-propanol, which was detected in SUMMATM samples at an average 0.026 ppmv, and in TST samples at 0.053 ppmv.

Jenkins et al. (1995) positively identified 26 of 27 target analytes in TST samples. Dichloromethane was the only TST target analyte not detected. Despite calibration of the instrument over about a 20-fold concentration range, only 11 of the target analytes were measured to be within the calibration range in all 3 TST samples. Tables 4-4 through 4-6 give the reported 3-sample average concentrations for 24 positively identified compounds. Quantitated compounds are given in Table 4-4, compounds for which the measurement in 1 or more samples was outside the instrument calibration range are given in Table 4-5, and compounds for which the ORNL practical holding time was exceeded are given in Table 4-6. Tables 4-4, 4-5, and 4-6 are mutually exclusive, so no compound appears in more than 1 of these tables. Note that 1 compound in Table 4-6, butanal, was quantitated in all 3 samples, but placed in Table 4-6 because it exceeded its practical holding time. Data in Tables 4-5 and 4-6 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 (Jenkins et al. 1995). The 3 compounds listed in Table 4-6 (butanal, 1-butanol, and 2-pentanone) had exceeded their practical holding times when the samples were analyzed 43 days after being collected. It should be noted that the practical holding times of some compounds are very short; butanal, for example, has a practical holding time of only 1 day.

Tributyl phosphate and dibutyl butylphosphonate were both positively identified by ORNL in one of the TST samples, but these results are suspect because of an apparent sampling manifold contamination

problem. Huckaby and Bratzel (1995b) briefly describe the evidence that tributyl phosphate and dibutyl butylphosphate were contaminants of several sampling events. Furthermore, because calibration of the instrumentation for these compounds requires special procedures and these compounds have other known sampling problems, quantitation was not attempted.

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 AX-102 and obtain concentration in ppmv of analyte in moist tank air, multiply by 0.969.

Collection of TST samples was conducted in a manner to minimize inter-laboratory differences. Specifically, identical sample volumes were drawn through like sets of TSTs (though the design of the TSTs used by the 2 laboratories is slightly different), and they were collected simultaneously from alternate locations of the sorbent trap sampling station of the VSS. Table 4-7 lists the 10 target analytes that were common to both ORNL and PNL analyses, with their measured concentrations in PNL SUMMA™ samples, PNL TST samples, and ORNL TST samples. Comparison of the data given in Table 4-7 suggests the 3 sampling and analysis methodologies are in very good agreement. No consistent laboratory or sample device bias is indicated by the data given in Table 4-7.

Four positively identified analytes in tank AX-102 were measured to be above 0.1 ppmv: 1-butanol, propanone (acetone), ethanenitrile (acetonitrile), and trichlorofluoromethane. At the reported concentrations, these headspace constituents 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 SUMMA™ 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 SUMMA™ samples has been problematic.

The lists of tentatively identified compounds recovered from PNL SUMMA™ and PNL TST samples with their estimated concentrations, are given in Tables 4-8 and 4-9, respectively. Compounds are listed in these tables in the order in which they eluted chromatographically, and only non-zero results are included in the reported averages. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The list of tentatively identified compounds detected in ORNL TST samples, and their estimated concentrations, is given in Table 4-10. Compounds in Table 4-10 are also listed in the order in which the eluted chromatographically. The averages reported by ORNL in Table 4-10 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. Because the ORNL list of tentatively identified compounds is long and locating any given compound may be difficult, it has been sorted alphanumerically by compound name in Table 4-11, and by estimated concentration in Table 4-12. Numbers in the first column of Tables 4-11 and 4-12 (Cmpd #) refer to the location of the compound in Table 4-10. Estimated concentrations are in mg/m³, based on dry air at 0 °C and 1.01 bar.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995) and Clauss et al. (1995), respectively, and should be reviewed before this data is used for decision making. Concentrations given in Tables 4-8 through and 4-12 should be considered estimates.

4.3 Discussion of Organic Compounds

Some of the organic compounds identified in the June 1995 tank AX-102 headspace samples are apparently from residual organic solvents still present in the tank waste. In particular, the semivolatile straight-chain alkanes 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). Tributyl phosphate itself was detected by ORNL in TST samples, as well as dibutyl butylphosphonate, a common contaminant present from the manufacture of tributyl phosphate, but these may also have been present in the TST samples because of a sampling manifold contamination problem. It is also likely that the tentatively identified semivolatile branched alkanes were also introduced with the NPHs as waste.

The concentrations of the NPHs in the tank AX-102 headspace are too high and the solubilities of the NPHs in aqueous wastes are too small to assume that they are dissolved in the aqueous waste of tank AX-102. An organic liquid phase of some sort probably exists, though whether it resides as a small puddle or is lightly smeared over different parts of the tank and waste can not be determined from vapor samples. The headspace concentrations of these semivolatile constituents depend on the amount of organic-phase surface area, the temperature of the organic-phase, and the ventilation rate of the tank.

Though the NPHs are not present at high concentrations in the headspace of tank AX-102, they are thought to be the precursors of most of the other organic compounds identified in tank AX-102. Condensed phase chemical and radiolytic reactions degrade the NPHs into shorter carbon chain molecules, such as the volatile nitriles, aldehydes, alcohols, and alkenes. The abundance of these in the headspace probably depends on their generation rates and the tank ventilation rate, because they are relatively volatile, and probably do not remain in the organic liquid phase in significant concentrations. Other degradation products of the NPHs may include non-volatile acids (which would be converted to salts on contact with the aqueous waste), and high-molecular weight compounds with very low volatilities.

Tetrachloroethene, a chlorinated solvent, was positively identified in the tank AX-102 samples. This common cleaning solvent may have been added to the tank in small quantities when it became radiologically contaminated. The other positively identified halogenated compound, trichlorofluoromethane, is a freon (and not really a solvent), with a boiling point of about 23 °C. The source of this is not known, but it is frequently detected in the waste tank headspaces. One plausible explanation for its presence is that it was the gas component of urethane foam that was used to seal

concrete pit covers on the tanks. Whether this type of foam was used on tank AX-102 has not been determined.

The total organic vapor concentration in PNL TST and SUMMATM canister samples was determined (by GC/MS) to be 7.38 mg/m³ and 9.90 mg/m³, respectively (Clauss et al. 1995). These estimates differ primarily because of the relatively high concentration of methanol, 4.0 mg/m³, found in SUMMATM canister samples. Methanol in PNL TSTs was estimated to be only 0.42 mg/m³, and a plausible explanation is that methanol is not well retained (trapped) by TSTs (the ORNL methanol estimate is also low, 0.79 mg/m³). A similar summation of quantitative, semiquantitative, and estimated organic vapor concentrations reported by ORNL from TST analyses (also by GC/MS) gave an estimated 7.6 mg/m³ of organic vapors (Jenkins et al. 1995). The PNL TST and ORNL TST estimates of total organic vapor concentration are in excellent agreement.

In general, the organic vapors in tank AX-102 are similar to those observed in other passively ventilated waste tanks at the Hanford site. The estimated total organic vapor concentration, ranging from 7.38 to 9.90 mg/m³, is typical for the passively ventilated tanks that have been sampled.

5.0 SUMMARY

The tank AX-102 headspace was sampled in June 1995 for gases and vapors to address flammability and industrial hygiene concerns. Results of sample collection and analysis have been reported. It was determined that no headspace constituents exceeded the flammability or industrial hygiene notification limits specified in the current *Vapor Sampling and Analysis Plan* (Homi 1995b).

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Table 2-1
Tank AX-102 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 blanks + 3 field blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks + 3 field blanks
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks + 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

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Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
	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
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table 3-1
 Tank AX-102 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	34	9	9
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	704	6	0.9
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 98	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.18	0.03	7
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.08	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	50	0.6	1
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	16,400 (11.9 mg/L)	700 (0.5 mg/L)	4

¹ CAS = Chemical Abstracts Service.

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

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Table 4-1
Tank AX-102 Quantitatively Measured 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	0.26	0.03	12
2	Propanone (acetone)	67-64-1	0.22	0.02	9
3	Trichlorofluoromethane	75-69-4	0.40	0.04	10
4	Propanenitrile	107-12-0	0.045	0.004	9
5	1-Propanol	71-23-8	0.026	0.002	8
6	2-Butanone	78-93-3	0.043	0.004	9
7	n-Butanenitrile	109-74-0	0.088	0.007	8
8	n-Heptane	142-82-5	0.011	0.001	9
9	Tetrachloroethylene	127-18-4	0.024	0.001	4
10	Methane	74-82-8	< 12	--	--

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 AX-102 Quantitatively Measured Compounds in TST 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	0.16	0.003	2
2	Propanone (acetone)	67-64-1	0.17	0.01	7
3	Trichlorofluoromethane	75-69-4	0.25	0.001	1
4	Dichloromethane (methylene chloride)	75-09-2	0.0063	0.0007	12
5	Propanenitrile	107-12-0	0.075	0.008	11
6	1-Propanol	71-23-8	0.053	0.005	9
7	2-Butanone	78-93-3	0.051	0.001	1
8	n-Butanenitrile	109-74-0	0.085	0.001	1
9	n-Heptane	142-82-5	0.014	0.0003	2
10	Toluene	108-88-3	0.0055	0.0004	7
11	Tetrachloroethylene	127-18-4	0.025	0.001	2

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 4-3
Tank AX-102 Comparison of Organic Compounds in TST and SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Compound	CAS ¹ Number	TST Average ² (ppmv)	SUMMA™ Average ³ (ppmv)	RPD ⁴ (%)
Ethanenitrile (acetonitrile)	75-05-8	0.16	0.26	-48
Propanone (acetone)	67-64-1	0.17	0.22	-26
Trichlorofluoromethane	75-69-4	0.25	0.40	-46
Dichloromethane (methylene chloride)	75-09-2	0.0063	< 0.005	—
Propanenitrile	107-12-0	0.075	0.045	50
1-Propanol	71-23-8	0.053	0.026	68
2-Butanone	78-93-3	0.051	0.043	17
n-Butanenitrile	109-74-0	0.085	0.088	-3
n-Heptane	142-82-5	0.014	0.011	24
Toluene	108-88-3	0.0055	< 0.005	—
Tetrachloroethylene	127-18-4	0.025	0.024	4

1 CAS = Chemical Abstract Service.

2 Average of 3 TST sample analyses by PNL.

3 Average of 3 SUMMA™ sample analyses by PNL.

4 RPD = relative percent difference (i.e., the difference divided by the mean of the 2 values).

Table 4-4
Tank AX-102 Quantitatively Measured Organic Analytes 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	0.15	0.07	41
2	Propanone (acetone)	67-64-1	0.11	0.04	41
3	n-Butanenitrile	109-74-0	0.090	0.021	24
4	n-Heptane	142-82-5	0.017	0.004	21
5	n-Pentanenitrile	110-59-8	0.016	0.003	16
6	2-Hexanone	591-78-6	0.011	0.001	12
7	2-Heptanone	110-43-0	0.014	0.002	18
8	n-Undecane	1120-21-4	0.0039	0.0002	5
9	n-Dodecane	112-40-3	0.0091	0.0008	9
10	n-Tridecane	629-50-5	0.036	0.006	17

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

Table 4-5
Tank AX-102 Positively Identified Organic Analytes in TST Samples--
Analyses by Oak Ridge National Laboratory¹

Cmpd #	Compound	CAS ² Number	Average ³ (ppmv)	Standard Deviation (ppmv)	RSD ⁴ (%)
1	1,1-Dichloroethene (vinylidene chloride)	75-35-4	0.0033	0.0012	37
2	Propanenitrile	107-12-0	0.048	0.014	28
3	n-Hexane	110-54-3	0.0047	0.0013	28
4	Benzene	71-43-2	0.0019	0.0003	16
5	Toluene	108-88-3	0.0038	0.0007	18
6	n-Octane	111-65-9	0.0025	0.0003	13
7	n-Hexanenitrile	628-73-9	0.0041	0.0008	18
8	n-Nonane	111-84-2	0.0017	0.0003	18
9	n-Heptanenitrile	629-08-3	0.0029	0.0007	23
10	2-Octanone	111-13-7	0.0017	0.0007	40
11	n-Decane	124-18-5	0.0021	0.0001	6

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, 1-L TST samples.

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

Table 4-6
Tank AX-102 Positively Identified Organic Analytes 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	0.088	0.032	36
2	1-Butanol ⁶	71-36-3	0.17	0.04	26
3	2-Pentanone ⁶	107-87-9	0.0073	0.0017	23

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

2 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples.

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

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

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

Table 4-7
Tank AX -102 Comparison of Positively Identified Organic Compounds --
Analyses by Pacific Northwest Laboratory
and Oak Ridge National Laboratory

Compound	CAS ¹ Number	PNL SUMMA™ Average ² (ppmv)	PNL TST Average ³ (ppmv)	ORNL TST Average ⁴ (ppmv)
Ethanenitrile (acetonitrile)	75-05-8	0.26	0.16	0.15
Propanone (acetone)	67-64-1	0.22	0.17	0.11
1,1-Dichloroethene	75-35-4	< 0.005	< 0.005	0.0033 ⁵
Dichloromethane (methylene chloride)	75-09-2	< 0.005	0.0063	< 0.0053
Propanenitrile	107-12-0	0.045	0.075	0.048 ⁵
n-Butanenitrile	109-74-0	0.088	0.085	0.090
Benzene	71-43-2	< 0.005	< 0.005	0.0019 ⁵
n-Heptane	142-82-5	0.011	0.014	0.017
Toluene	108-88-3	< 0.005	0.0055	0.0038 ⁵
n-Decane	124-18-5	< 0.005	< 0.005	0.0021 ⁵

1 CAS = Chemical Abstract Service.

2 Average of 3 SUMMA™ sample analyses by PNL.

3 Average of 3 TST sample analyses by PNL.

4 Average of 3, 1-L TST sample analyses by ORNL.

5 This compound was not quantitated in all 3 TST samples.

Table 4-8
Tank AX-102 Tentatively Identified Compounds in SUMMA™ Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Propane	74-98-6	0.24	0.02
2	Unknown		0.076	0.026
3	Methanol (methyl alcohol)	67-56-1	4.0	0.4
4	n-Butane	106-97-8	0.28	0.03
5	Methane, dichlorofluoro-	75-43-4	0.25	0.04
6	Ethanol	64-17-5	0.47	0.24
7	Butanal	123-72-8	0.22	0.02
8	Unknown		0.059	0.013
9	1-Butanol	71-36-3	0.39	0.03
10	Unknown		0.14	0.01
11	Unknown Alkane		0.051	0.001
12	Unknown		0.049	0.003
13	4-Heptanone	123-19-3	< 0.05	--
14	3-Heptanone	106-35-4	1.2	0.2
15	2-Heptanone ³	110-43-0	0.049	--
16	Unknown		0.042	0.011
17	Unknown Aldehyde		0.071	0.013
18	Unknown		0.16	0.01
Sum of tentatively identified compounds:			7.7	

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 samples. Values given are estimates.

3 Detected in only 1 sample.

Table 4-9
Tank AX-102 Tentatively Identified Compounds in TST Samples --
Analyses by Pacific Northwest Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard ³ Deviation (mg/m ³)
1	Methanol (methyl alcohol)	67-56-1	0.42	0.05
2	n-Butane	106-97-8	0.047	0.006
3	Ethanol	64-17-5	0.12	0.01
4	1-Propanol	71-23-8	0.10	0.03
5	Unknown Ketone		0.049	0.011
6	Butanal	123-72-8	0.073	0.041
7	Unknown Aldehyde		0.050	0.008
8	Propylene Glycol	57-55-6	0.14	0.01
9	Pentanenitrile	110-59-8	0.061	0.017
10	2-Hexanone ⁴	591-78-6	0.051	0.004
11	Heptane, 3-methyl-	589-81-1	0.079	0.003
12	Unknown		0.035	0.018
13	Nitric acid, butyl ester	928-45-0	0.061	0.007
14	Butane, 1-nitro- ⁵	627-05-4	0.049	--
15	3-Heptanone	106-35-4	1.3	0.03
16	3-Heptanol	589-82-2	0.13	0.002
17	Butanamide	541-35-5	0.079	0.023
18	Unknown		0.067	0.004
19	Unknown		0.096	0.002
20	Hexanal, 2-ethyl-	123-05-7	0.11	0.01
21	Unknown		0.030	0.031
22	Unknown		0.039	0.011
23	Unknown		0.18	0.02
24	1-Hexanol, 2'-ethyl-	104-76-7	0.14	0.01
25	Unknown Alcohol		0.18	0.001
26	Unknown Ketone		0.073	0.002

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard ³ Deviation (mg/m ³)
27	n-Dodecane	112-40-3	0.084	0.002
28	n-Tridecane	629-50-5	0.22	0.003
29	n-Tetradecane	629-59-4	0.091	0.001
Sum of tentatively identified compounds:			4.1	

1 CAS = Chemical Abstract Service.

2 Based on analyses of 3 TST samples. Values given are estimates.

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

4 Detected in only 2 samples.

5 Detected in only 1 sample.

Table 4-10
Tank AX-102 Tentatively Identified Organic Compounds in TST Samples
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
1	Methyl nitrite	624-91-9	0.027	0.029
2	Methanol (methyl alcohol)	67-56-1	0.79	0.28
3	Mixture		0.0085	0.0090
4	Methane, dichlorofluoro-	75-43-4	0.038	0.015
5	Ethanol	64-17-5	0.13	0.05
6	Trichloromonofluoromethane	75-69-4	0.34	0.08
7	Silane, chlorotrimethyl-	75-77-4	0.016	0.028
8	Formamide and others		0.0043	0.0074
9	Mixture		0.010	0.010
10	1-Propanol	71-23-8	0.061	0.013
11	3-Buten-2-one	78-94-4	0.029	0.008
12	2-Butanone	78-93-3	0.14	0.04
13	Nitric acid, ethyl ester	625-58-1	0.035	0.018
14	Cyclopropane, butyl-	930-57-4	0.0022	0.0038
15	1,4-Butanediol, dinitrate	3457-91-8	0.035	0.006
16	Alkene		0.0074	0.0068
17	Propane, 1-nitro-	108-03-2	0.021	0.010
18	Pyrazine	290-37-9	0.0029	0.0051
19	Propylene Glycol	57-55-6	0.053	0.038
20	Heptane, 3-methyl-	589-81-1	0.036	0.005
21	1-Octene	111-66-0	0.0024	0.0042
22	Benzothiazole, 2-phenyl-	883-93-2	0.0069	0.0119
23	3-Hexanone	589-38-8	0.018	0.010
24	Cyclopentane, 1,2,3-trimethyl-	2815-57-8	0.0016	0.0027
25	2-Ethyl-5-methylfuran	1703-52-2	0.0078	0.0136
26	Hexanal	66-25-1	0.018	0.017
27	Acetamide	60-35-5	0.0056	0.0065

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
28	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.0018	0.0031
29	Tetrachloroethylene	127-18-4	0.13	0.01
30	Cyclotrisiloxane, hexamethyl-	541-05-9	0.048	0.052
31	1,4-Butanediol, dinitrate	3457-91-8	0.046	0.007
32	3-Hexanone, 5-methyl-	623-56-3	0.0059	0.0052
33	Propane, 2-methyl-2-nitro-	594-70-7	0.051	0.016
34	Mixture		0.0025	0.0043
35	7-Oxabicyclo[4.1.0]heptane, 1-methyl-	1713-33-3	0.0071	0.0062
36	Nonanal	124-19-6	0.0064	0.0058
37	4-Heptanone	123-19-3	0.086	0.009
38	Alkylcyclopropane		0.0035	0.0060
39	3-Hexanone, 2,5-dimethyl-	1888-57-9	0.033	0.014
40	3-Heptanone	106-35-4	0.98	0.10
41	3-Heptanol	589-82-2	0.092	0.011
42	Heptanal	111-71-7	0.0073	0.0063
43	Furan, 2,3-dihydro-4-(1-methylpropyl)-,(S)-	34379-54-9	0.0018	0.0032
44	Pyridine, 2-ethyl-	100-71-0	0.0072	0.0063
45	Butyrolactone	96-48-0	0.012	0.002
46	Mixture		0.0205	0.0020
47	3-Hexanone, 4-ethyl-	6137-12-8	0.0011	0.0019
48	2,5-Hexanedione	110-13-4	0.0026	0.0044
49	2,2'-Bioxepane	74793-02-5	0.036	0.031
50	3-Hexen-2-one	763-93-9	0.016	0.028
51	3-Penten-2-one, 4-methyl-	141-79-7	0.086	0.009
52	Hexanal, 2-ethyl-	123-05-7	0.13	0.11
53	3-Hepten-2-one, 3-methyl-	39899-08-6	0.048	0.083
54	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	0.044	0.006
55	Butanamide	541-35-5	0.0053	0.0092
56	3-Hexen-2-one, 5-methyl-	5166-53-0	0.017	0.004

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
57	4-Octanone	589-63-9	0.0072	0.0064
58	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.0014	0.0025
59	Cyclotetrasiloxane, octamethyl-	556-67-2	0.022	0.031
60	3-Methyl-4-octanone	20754-04-5	0.012	0.011
61	2-Hexenal, 2-ethyl-	645-62-5	0.017	0.004
62	5-Hexen-1-ol	821-41-0	0.071	0.003
63	Mixture		0.0042	0.0048
64	Hexane, 2,5-dimethyl-	592-13-2	0.23	0.02
65	Pyridine, 5-ethyl-2-methyl-	104-90-5	0.0018	0.0030
66	Mixture		0.0023	0.0040
67	1-Propanol, 2,2-dimethyl-, nitrate	926-42-1	0.17	0.01
68	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.011	0.001
69	5-Nonanone	502-56-7	0.0016	0.0028
70	Acetophenone and alkene		0.022	0.002
71	Octanenitrile	124-12-9	0.0029	0.0051
72	Mixture		0.0014	0.0025
73	2-Nonanone	821-55-6	0.0027	0.0048
74	Nonanal and others		0.012	0.002
75	Alkyl Nitrile		0.014	0.000
76	Nitric acid, pentyl ester	1002-16-0	0.0016	0.0027
77	Alkyl Nitrile		0.0025	0.0044
78	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.0071	0.0074
79	Propanoic acid, 2-methyl-, butyl ester	97-87-0	0.017	0.016
80	Decane, 2,2,3-trimethyl-	62338-09-4	0.014	0.001
81	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	0.0071	0.0062
82	5-Undecanone, 2-methyl-	50639-02-6	0.0016	0.0028
83	2,4(3H,5H)-Furandione, 3-methyl-	1192-51-4	0.018	0.003
84	2-Pyrrolidinone and others		0.10	0.00

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
85	Alkanal and others		0.032	0.008
86	Alkene		0.0017	0.0030
87	Alkene		0.0024	0.0042
88	Mixture		0.0013	0.0022
89	Mixture		0.0011	0.0019
90	Methenamine	100-97-0	0.0038	0.0066
91	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	0.015	0.006
92	Mixture		0.0037	0.0064
93	Butyl, 2-ethylhexanoate	68443-63-0	0.0071	0.0064
94	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	27750-45-4	0.0038	0.0066
95	6-Dodecanone and others		0.0036	0.0063
96	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	0.0020	0.0035
97	3,6-Dioxo-2,4,5,7-tetrasilaooctane, 2,2,4,4,5,5,7,7-octamethyl-	4342-25-0	0.021	0.003
98	Tetradecane	629-59-4	0.12	0.01
99	6-Tridecanone	22026-12-6	0.0034	0.0059
100	5-Tridecanone	30692-16-1	0.020	0.018
101	2(3H)-Furanone, 5-hexyldihydro-	706-14-9	0.0011	0.0018
102	3-Tridecanone	1534-26-5	0.011	0.010
103	Pentadecane	629-62-9	0.010	0.012
104	1,1'-Biphenyl, 2-chloro-	2051-60-7	0.0023	0.0040
105	Heptasiloxane, hexadecamethyl-	541-01-5	0.022	0.002
106	6-Dodecanone	6064-27-3	0.0072	0.0063
107	3-Tridecanone	1534-26-5	0.0043	0.0075
108	2-Tetradecanone	2345-27-9	0.0056	0.0053
109	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.0016	0.0028
110	Benzenesulfonamide, N-butyl-	3622-84-2	0.18	0.13

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
Sum of tentatively identified compounds:			5.0	

1 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples. Values given are estimates.

Table 4-11
Tank AX-102 Tentatively Identified Organic Compounds in TST Samples
Sorted Alphanumerically by Compound Name --
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
21	1-Octene	111-66-0	0.0024	0.0042
10	1-Propanol	71-23-8	0.061	0.013
67	1-Propanol, 2,2-dimethyl-, nitrate	926-42-1	0.17	0.01
104	1,1'-Biphenyl, 2-chloro-	2051-60-7	0.0023	0.0040
31	1,4-Butanediol, dinitrate	3457-91-8	0.046	0.007
15	1,4-Butanediol, dinitrate	3457-91-8	0.035	0.006
73	2-Nonanone	821-55-6	0.0027	0.0048
84	2-Pyrrolidinone and others		0.10	0.00
12	2-Butanone	78-93-3	0.14	0.04
61	2-Hexenal, 2-ethyl-	645-62-5	0.017	0.004
108	2-Tetradecanone	2345-27-9	0.0056	0.0053
25	2-Ethyl-5-methylfuran	1703-52-2	0.0078	0.0136
49	2,2'-Bioxepane	74793-02-5	0.036	0.031
48	2,5-Hexanedione	110-13-4	0.0026	0.0044
83	2,4(3H,5H)-Furandione, 3-methyl-	1192-51-4	0.018	0.003
96	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	0.0020	0.0035
68	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.011	0.001
54	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	0.044	0.006
81	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	0.0071	0.0062
101	2(3H)-Furanone, 5-hexyldihydro-	706-14-9	0.0011	0.0018
28	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.0018	0.0031
91	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	0.015	0.006
11	3-Buten-2-one	78-94-4	0.029	0.008
107	3-Tridecanone	1534-26-5	0.0043	0.0075
102	3-Tridecanone	1534-26-5	0.011	0.010
60	3-Methyl-4-octanone	20754-04-5	0.012	0.011

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
23	3-Hexanone	589-38-8	0.018	0.010
51	3-Penten-2-one, 4-methyl-	141-79-7	0.086	0.009
32	3-Hexanone, 5-methyl-	623-56-3	0.0059	0.0052
47	3-Hexanone, 4-ethyl-	6137-12-8	0.0011	0.0019
53	3-Hepten-2-one, 3-methyl-	39899-08-6	0.048	0.083
56	3-Hexen-2-one, 5-methyl-	5166-53-0	0.017	0.004
50	3-Hexen-2-one	763-93-9	0.016	0.028
41	3-Heptanol	589-82-2	0.092	0.011
40	3-Heptanone	106-35-4	0.98	0.10
39	3-Hexanone, 2,5-dimethyl-	1888-57-9	0.033	0.014
97	3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-	4342-25-0	0.021	0.003
37	4-Heptanone	123-19-3	0.086	0.009
57	4-Octanone	589-63-9	0.0072	0.0064
82	5-Undecanone, 2-methyl-	50639-02-6	0.0016	0.0028
62	5-Hexen-1-ol	821-41-0	0.071	0.003
100	5-Tridecanone	30692-16-1	0.020	0.018
69	5-Nonanone	502-56-7	0.0016	0.0028
95	6-Dodecanone and others		0.0036	0.0063
106	6-Dodecanone	6064-27-3	0.0072	0.0063
99	6-Tridecanone	22026-12-6	0.0034	0.0059
35	7-Oxabicyclo[4.1.0]heptane, 1-methyl-	1713-33-3	0.0071	0.0062
27	Acetamide	60-35-5	0.0056	0.0065
70	Acetophenone and alkene		0.022	0.002
85	Alkanal and others		0.032	0.008
16	Alkene		0.0074	0.0068
86	Alkene		0.0017	0.0030
87	Alkene		0.0024	0.0042
75	Alkyl Nitrile		0.014	0.000

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Cmpd #	Compound's	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
77	Alkyl Nitrile		0.0025	0.0044
38	Alkylcyclopropane		0.0035	0.0060
110	Benzenesulfonamide, N-butyl-	3622-84-2	0.18	0.13
78	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.0071	0.0074
22	Benzothiazole, 2-phenyl-	883-93-2	0.0069	0.0119
55	Butanamide	541-35-5	0.0053	0.0092
93	Butyl, 2-ethylhexanoate	68443-63-0	0.0071	0.0064
45	Butyrolactone	96-48-0	0.012	0.002
58	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.0014	0.0025
24	Cyclopentane, 1,2,3-trimethyl-	2815-57-8	0.0016	0.0027
14	Cyclopropane, butyl-	930-57-4	0.0022	0.0038
59	Cyclotetrasiloxane, octamethyl-	556-67-2	0.022	0.031
30	Cyclotrisiloxane, hexamethyl-	541-05-9	0.048	0.052
80	Decane, 2,2,3-trimethyl-	62338-09-4	0.014	0.001
5	Ethanol	64-17-5	0.13	0.05
8	Formamide and others		0.0043	0.0074
43	Furan, 2,3-dihydro-4-(1-methylpropyl)-,(S)-	34379-54-9	0.0018	0.0032
42	Heptanal	111-71-7	0.0073	0.0063
20	Heptane, 3-methyl-	589-81-1	0.036	0.005
105	Heptasiloxane, hexadecamethyl-	541-01-5	0.022	0.002
26	Hexanal	66-25-1	0.018	0.017
52	Hexanal, 2-ethyl-	123-05-7	0.13	0.11
64	Hexane, 2,5-dimethyl-	592-13-2	0.23	0.02
4	Methane, dichlorofluoro-	75-43-4	0.038	0.015
2	Methanol (methyl alcohol)	67-56-1	0.79	0.28
90	Methenamine	100-97-0	0.0038	0.0066
1	Methyl nitrite	624-91-9	0.027	0.029
3	Mixture		0.0085	0.0090

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
34	Mixture		0.0025	0.0043
46	Mixture		0.0205	0.0020
63	Mixture		0.0042	0.0048
66	Mixture		0.0023	0.0040
72	Mixture		0.0014	0.0025
88	Mixture		0.0013	0.0022
89	Mixture		0.0011	0.0019
9	Mixture		0.010	0.010
92	Mixture		0.0037	0.0064
13	Nitric acid, ethyl ester	625-58-1	0.035	0.018
76	Nitric acid, pentyl ester	1002-16-0	0.0016	0.0027
36	Nonanal	124-19-6	0.0064	0.0058
74	Nonanal and others		0.012	0.002
71	Octanenitrile	124-12-9	0.0029	0.0051
103	Pentadecane	629-62-9	0.010	0.012
17	Propane, 1-nitro-	108-03-2	0.021	0.010
33	Propane, 2-methyl-2-nitro-	594-70-7	0.051	0.016
94	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	27750-45-4	0.0038	0.0066
109	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1	0.0016	0.0028
79	Propanoic acid, 2-methyl-, butyl ester	97-87-0	0.017	0.016
19	Propylene Glycol	57-55-6	0.053	0.038
18	Pyrazine	290-37-9	0.0029	0.0051
44	Pyridine, 2-ethyl-	100-71-0	0.0072	0.0063
65	Pyridine, 5-ethyl-2-methyl-	104-90-5	0.0018	0.0030
7	Silane, chlorotrimethyl-	75-77-4	0.016	0.028
29	Tetrachloroethylene	127-18-4	0.13	0.01
98	Tetradecane	629-59-4	0.12	0.01

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
6	Trichloromonofluoromethane	75-69-4	0.34	0.08

1 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples. Values given are estimates.

Table 4-12
Tank AX-102 Tentatively Identified Organic Compounds in TST Samples
Sorted in Order of Decreasing Estimated Concentrations
Analyses by Oak Ridge National Laboratory

Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
40	3-Heptanone	106-35-4	0.98	0.10
2	Methanol (methyl alcohol)	67-56-1	0.79	0.28
6	Trichloromonofluoromethane	75-69-4	0.34	0.08
64	Hexane, 2,5-dimethyl-	592-13-2	0.23	0.02
110	Benzenesulfonamide, N-butyl-	3622-84-2	0.18	0.13
67	1-Propanol, 2,2-dimethyl-, nitrate	926-42-1	0.17	0.01
12	2-Butanone	78-93-3	0.14	0.04
29	Tetrachloroethylene	127-18-4	0.13	0.01
5	Ethanol	64-17-5	0.13	0.05
52	Hexanal, 2-ethyl-	123-05-7	0.13	0.11
98	Tetradecane	629-59-4	0.12	0.01
84	2-Pyrrolidinone and others		0.10	0.00
41	3-Heptanol	589-82-2	0.092	0.011
37	4-Heptanone	123-19-3	0.086	0.009
51	3-Penten-2-one, 4-methyl-	141-79-7	0.086	0.009
62	5-Hexen-1-ol	821-41-0	0.071	0.003
10	1-Propanol	71-23-8	0.061	0.013
19	Propylene Glycol	57-55-6	0.053	0.038
33	Propane, 2-methyl-2-nitro-	594-70-7	0.051	0.016
30	Cyclotrisiloxane, hexamethyl-	541-05-9	0.048	0.052
53	3-Hepten-2-one, 3-methyl-	39899-08-6	0.048	0.083
31	1,4-Butanediol, dinitrate	3457-91-8	0.046	0.007
54	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	0.044	0.006
4	Methane, dichlorofluoro-	75-43-4	0.038	0.015
49	2,2'-Bioxepane	74793-02-5	0.036	0.031
20	Heptane, 3-methyl-	589-81-1	0.036	0.005

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
13	Nitric acid, ethyl ester	625-58-1	0.035	0.018
15	1,4-Butanediol, dinitrate	3457-91-8	0.035	0.006
39	3-Hexanone, 2,5-dimethyl-	1888-57-9	0.033	0.014
85	Alkanal and others		0.032	0.008
11	3-Buten-2-one	78-94-4	0.029	0.008
1	Methyl nitrite	624-91-9	0.027	0.029
59	Cyclotetrasiloxane, octamethyl-	556-67-2	0.022	0.031
70	Acetophenone and alkene		0.022	0.002
105	Heptasiloxane, hexadecamethyl-	541-01-5	0.022	0.002
97	3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-	4342-25-0	0.021	0.003
17	Propane, 1-nitro-	108-03-2	0.021	0.010
46	Mixture		0.0205	0.0020
100	5-Tridecanone	30692-16-1	0.020	0.018
26	Hexanal	66-25-1	0.018	0.017
83	2,4(3H,5H)-Furandione, 3-methyl-	1192-51-4	0.018	0.003
23	3-Hexanone	589-38-8	0.018	0.010
61	2-Hexenal, 2-ethyl-	645-62-5	0.017	0.004
56	3-Hexen-2-one, 5-methyl-	5166-53-0	0.017	0.004
79	Propanoic acid, 2-methyl-, butyl ester	97-87-0	0.017	0.016
50	3-Hexen-2-one	763-93-9	0.016	0.028
7	Silane, chlorotrimethyl-	75-77-4	0.016	0.028
91	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	0.015	0.006
75	Alkyl Nitrile		0.014	0.000
80	Decane, 2,2,3-trimethyl-	62338-09-4	0.014	0.001
45	Butyrolactone	96-48-0	0.012	0.002
74	Nonanal and others		0.012	0.002
60	3-Methyl-4-octanone	20754-04-5	0.012	0.011
68	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.011	0.001

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
102	3-Tridecanone	1534-26-5	0.011	0.010
9	Mixture		0.010	0.010
103	Pentadecane	629-62-9	0.010	0.012
3	Mixture		0.0085	0.0090
25	2-Ethyl-5-methylfuran	1703-52-2	0.0078	0.0136
16	Alkene		0.0074	0.0068
42	Heptanal	111-71-7	0.0073	0.0063
44	Pyridine, 2-ethyl-	100-71-0	0.0072	0.0063
57	4-Octanone	589-63-9	0.0072	0.0064
106	6-Dodecanone	6064-27-3	0.0072	0.0063
81	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	0.0071	0.0062
93	Butyl, 2-ethylhexanoate	68443-63-0	0.0071	0.0064
78	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethylsilyl ester	3789-85-3	0.0071	0.0074
35	7-Oxabicyclo[4.1.0]heptane, 1-methyl-	1713-33-3	0.0071	0.0062
22	Benzothiazole, 2-phenyl-	883-93-2	0.0069	0.0119
36	Nonanal	124-19-6	0.0064	0.0058
32	3-Hexanone, 5-methyl-	623-56-3	0.0059	0.0052
27	Acetamide	60-35-5	0.0056	0.0065
108	2-Tetradecanone	2345-27-9	0.0056	0.0053
55	Butanamide	541-35-5	0.0053	0.0092
8	Formamide and others		0.0043	0.0074
107	3-Tridecanone	1534-26-5	0.0043	0.0075
63	Mixture		0.0042	0.0048
94	Propanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	27750-45-4	0.0038	0.0066
90	Methenamine	100-97-0	0.0038	0.0066
92	Mixture		0.0037	0.0064
95	6-Dodecanone and others		0.0036	0.0063

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
38	Alkylcyclopropane		0.0035	0.0060
99	6-Tridecanone	22026-12-6	0.0034	0.0059
18	Pyrazine	290-37-9	0.0029	0.0051
71	Octanenitrile	124-12-9	0.0029	0.0051
73	2-Nonanone	821-55-6	0.0027	0.0048
48	2,5-Hexanedione	110-13-4	0.0026	0.0044
34	Mixture		0.0025	0.0043
77	Alkyl Nitrile		0.0025	0.0044
87	Alkene		0.0024	0.0042
21	1-Octene	111-66-0	0.0024	0.0042
66	Mixture		0.0023	0.0040
104	1,1'-Biphenyl, 2-chloro-	2051-60-7	0.0023	0.0040
14	Cyclopropane, butyl-	930-57-4	0.0022	0.0038
96	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	0.0020	0.0035
65	Pyridine, 5-ethyl-2-methyl-	104-90-5	0.0018	0.0030
28	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	0.0018	0.0031
43	Furan, 2,3-dihydro-4-(1-methylpropyl)-, (S)-	34379-54-9	0.0018	0.0032
86	Alkene		0.0017	0.0030
109	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1, 3-propanediyl ester	74381-40-1	0.0016	0.0028
24	Cyclopentane, 1,2,3-trimethyl-	2815-57-8	0.0016	0.0027
69	5-Nonanone	502-56-7	0.0016	0.0028
82	5-Undecanone, 2-methyl-	50639-02-6	0.0016	0.0028
76	Nitric acid, pentyl ester	1002-16-0	0.0016	0.0027
58	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.0014	0.0025
72	Mixture		0.0014	0.0025
88	Mixture		0.0013	0.0022
47	3-Hexanone, 4-ethyl-	6137-12-8	0.0011	0.0019

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Cmpd #	Compounds	CAS ¹ Number	Average ² (mg/m ³)	Standard Deviation (mg/m ³)
89	Mixture		0.0011	0.0019
101	2(3H)-Furanone, 5-hexyldihydro-	706-14-9	0.0011	0.0018

1 CAS = Chemical Abstract Service.

3 Average of 3, 1-L TST samples. Values given are estimates.

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