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Tank 241-C-111 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-425)		ECN No. 623548

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
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ENGINEERING CHANGE NOTICE

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1. ECN No 623548

Proj. ECN

2. ECN Category (mark one)	3. Originator's Name, Organization, MSIN, and Telephone No.	3a. USQ Required?	4. Date
Supplemental [] Direct Revision [X] Change ECN [] Temporary [] Standby [] Supersedure [] Cancel/Void []	J. W. Osborne/Vapor Sampling/ S7-15/3-5379	[] Yes [X] No	May 31, 1995
	5. Project Title/No./Work Order No.	6. Bldg./Sys./Fac. No.	7. Approval Designator
	Vapor Sampling	200 Gen	N/A
	8. Document Numbers Changed by this ECN (includes sheet no. and rev.)	9. Related ECN No(s).	10. Related PO No.
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11a. Modification Work	11b. Work Package No.	11c. Modification Work Complete	11d. Restored to Original Condition (Temp. or Standby ECN only)
[] Yes (fill out Blk. 11b) [X] No (NA Blks. 11b, 11c, 11d)	N/A	N/A Cog. Engineer Signature & Date	N/A Cog. Engineer Signature & Date

12. Description of Change

Addition of caveat regarding Oak Ridge National Laboratory quality assurrance assessment in the organic vapor chapter. Minor editorial changes also.

13a. Justification (mark one)

Criteria Change	[]	Design Improvement	[]	Environmental	[]	Facility Deactivation	[]
As-Found	[]	Facilitate Const	[]	Const. Error/Omission	[]	Design Error/Omission	[X]

13b. Justification Details

New information regarding Oak Ridge National Laboratory analytical results pertaining to document was added.

14. Distribution (include name, MSIN, and no. of copies)

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1. ECN (use no. from pg. 1) 623548

15. Design Verification Required	16. Cost Impact				17. Schedule Impact (days)	
	ENGINEERING		CONSTRUCTION			
[] Yes	Additional	[] $	Additional	[] $	Improvement	[]
[X] No	Savings	[] $	Savings	[] $	Delay	[]

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

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

Document Number/Revision	Document Number/Revision	Document Number Revision

20. Approvals

Signature	Date	Signature	Date
OPERATIONS AND ENGINEERING		ARCHITECT-ENGINEER	
Cog. Eng. J. W. Osborne	5-31-95	PE	
Cog. Mgr. T. J. Kelley	5-31-95	QA	
QA		Safety	
Safety		Design	
Environ.		Environ.	
Other		Other	
		DEPARTMENT OF ENERGY	
		Signature or a Control Number that tracks the Approval Signature	
		ADDITIONAL	

RELEASE AUTHORIZATION

Document Number:	WHC-SD-WM-ER-425, REV 1
Document Title:	Tank 241-C-111 Vapor Sampling and Analysis Tank Characterization Report
Release Date:	5/31/95

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

APPROVED FOR PUBLIC RELEASE

WHC Information Release Administration Specialist:

Kara M. Broz — May 31, 1995

SUPPORTING DOCUMENT

1. Total Pages 18

2. Title	3. Number	4. Rev No.
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5. Key Words	6. Author
241-C-111, Headspace vapor samples, organic analytes, VSS, SUMMA™, inorganic gases and vapors	Name: J. L. Huckaby Signature Organization/Charge Code 75600/N4AB1

7. Abstract

Tank 241-C-111 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. 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 241-C-111 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).

8. RELEASE STAMP

RECORD OF REVISION	(1) Document Number WHC-SD-WM-ER-425	Page 1

(2) Title

Tank 241-C-111 Vapor Sampling and Analysis Tank Characterization Report

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release	
		(5) Cog. Engr.	(6) Cog. Mgr. Date
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~~BB~~ 1	(7) Made editorial changes and added information in organic vapor chapter.	J.W.Osborne	T.J.Kelley 5-31-95
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Tank 241-C-111 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank C-111 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. 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 C-111 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 C-111. Almost all of the data in this report was obtained from samples collected on September 13, 1994. Data from 2 other sets of samples, collected on August 10, 1993 and June 20, 1994, are in generally good agreement with the more recent data. The August 10, 1993 sample analyses have been summarized by Huckaby (1994), and the June 20, 1994 sample analyses are given by Ligotke et al. (1995).

X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank C-111 using the vapor sampling system (VSS) on September 13, 1994 by WHC Sampling and Mobile Laboratories, (WHC 1995). Sample collection and analysis were performed as directed by the sample and analysis plan (WHC 1995, Appendix A). The tank headspace temperature was determined to be 27 °C. Air from the tank C-111 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 6, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories (SNL). The 39 tank air samples and 2 ambient air control samples collected are listed in Table X-1 by analytical laboratory. Table X-1 also lists the 14 trip blanks provided by the laboratories.

A general description of vapor sampling and sample analysis methods is given by Huckaby (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 1995 and references therein.

X.2 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA™,[1] canister tank air samples for selected inorganic gases and vapors are given in Table X-2 in parts per million by volume (ppmv). Inorganic analyte sorbent traps were prepared and analyzed by PNL. SUMMA™ canisters were analyzed for inorganic analytes by OGIST. Reports by PNL (Lucke et al. 1995) and SNL/OGIST (Rasmussen 1994a) describe sample preparation and analyses.

The small relative standard deviations of the results, given in the last column in Table X-2, indicate the precision of reported results is good. Relative standard deviations range from 0.5 % for nitrous oxide results, to 16 % for ammonia and hydrogen results. 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.), and the small relative standard deviations suggest a high degree of control was maintained both in the field and in the laboratories.

X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 5.6 ppmv, is lower than the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995). Ammonia concentrations have typically been observed to be higher than this level in the waste tank headspaces. The relatively low ammonia concentration in tank C-111 may be related to the fact that only a small quantity of relatively cool waste is stored in tank C-111.

Hydrogen and nitrous oxide are commonly detected gases in the waste tanks. Believed to be products of chemical reactions and radiolysis of the waste, they have been found above the 1 ppmv level in virtually all the tank headspaces sampled to date. In general, hydrogen is of concern as a fuel. The measured 12.4 ppmv of hydrogen in tank C-111, however, represents only about 0.03 % of the lower flammability limit (LFL) for hydrogen in air, and is not a flammability concern at this level. The nitrous oxide concentration in tank C-111, 99.3 ppmv, is about 4 times the NIOSH 8-hr REL of 25 ppmv (NIOSH 1995).

X.2.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 198 ppmv, is about half of the normal ambient air concentration of about 400 ppmv. Lower than ambient carbon dioxide concentrations are expected. 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. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial

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

liquid, and condensate) in the tank. Compared to other waste tanks sampled to date, tank C-111 has a relatively high carbon dioxide concentration. For comparison, the carbon dioxide concentrations of the cascaded tanks BY-104, BY-105, and BY-106 are 10.5 ppmv, 94 ppmv, and 47.6 ppmv, respectively (Rasmussen 1994b, 1994c, 1994d).

Carbon monoxide in the tank C-111 headspace, at about 0.10 ppmv, is about normal for ambient air, where it typically ranges from 0.05 to 0.15 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common (e.g., carbon monoxide concentration in tank C-103 was 26.7 ppmv, Huckaby and Story 1994), and are thought to be due to the decomposition of organic waste in the tanks. The fact that tank C-111 does not have an elevated carbon monoxide concentration is an indication that tank C-111 lacks certain characteristics needed for carbon monoxide production. The low reported carbon monoxide concentration correlates well with the very low concentration of organic vapors in tank C-111 (see section X.3.3).

X.2.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium

Nitric oxide and nitrogen dioxide concentrations in the tank C-111 headspace were determined to be 0.62 ppmv and ≤ 0.08 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-111. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. The NIOSH 8-hr REL is 25 ppmv for nitric oxide, and the 15-minute short term exposure limit (STEL) for nitrogen dioxide is 1 ppmv.

The water vapor concentration of tank C-111 was determined to be about 22.2 mg/L, at the tank headspace temperature of 27 °C and pressure of 988 mbar (741 torr), (WHC 1995). This corresponds to water vapor partial pressure of 30.72 mbar (23.1 torr), to a dew point of 24.5 °C, and to a relative humidity of 86 %.

Tritium was tested for using silica gel sorbent traps. 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. Analysis of the silica gel indicated the total activity of the headspace to be below 50 pCi/L (WHC 1995).

X.3 ORGANIC VAPORS

Organic vapors in the tank C-111 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. None of the positively or tentatively identified organic analytes were at or above levels of concern. Both laboratories used gas chromatography and mass spectrometry to separate, identify, and quantitate

the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994) and Lucke et al. (1995). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIST (EPA 1988, Rasmussen 1994a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-111. 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.

X.3.1 Positively Identified Organic Analytes

ORNL positively identified 14 of 27 target analytes selected by WHC, (13 analytes were below detection limits). These analytes, and their average concentrations from the analysis of 3 TSTs, are given in Table X-3. The 27 TST target analytes for tank C-111 were based on the tank C-103 target analytes, which were selected by a PNL panel of toxicology experts as being of potential toxicological concern (Mahlum et al. 1994). Of the 14 analytes positively identified by ORNL, only acetonitrile, acetone, and dichloromethane were within the calibration range of the method. The other 11 target analytes were positively identified but were below the lower calibration limit. These concentrations are known with much greater certainty than the concentrations of tentatively identified compounds in Table X-5, but are not technically quantitative.

Also given in Table X-3 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL and OGIST. PNL performed analyses according to the EPA TO-14 methodology (EPA 1988, Lucke et al. 1995). None of the 40 TO-14 analytes was observed to be above the 0.002 ppmv quantitation limit of the analyses (Lucke et al. 1995 provide the complete TO-14 analyte list). The results for methane are those of OGIST (Rasmussen 1994a). Averages reported are from analyses of 3 SUMMA™ canister samples.

Three target analytes were common to both the ORNL and PNL analyses: dichloromethane, benzene, and toluene. The average dichloromethane concentration reported by ORNL, 0.18 ppmv, is not supported by PNL analyses. Given that PNL found no dichloromethane, and that the observed dichloromethane concentration in TSTs varied widely (i.e., the 3 TST results were 0.0045, 0.11, and 0.43 ppmv; Jenkins et al. 1994), it is likely the ORNL result is the result of contamination, and is in error. ORNL detected trace amounts of benzene and toluene, but these were both below the limit of detection of PNL (0.002 ppbv).

Except for dichloromethane, the 2 most abundant analytes in Table X-3 are methane and acetonitrile. At 0.32 ppmv, the methane concentration in tank C-111 is above ambient levels, which are typically about 0.2 ppmv. Elevated

methane concentrations have been observed in other waste tank headspaces, and methane is probably formed during the chemical and radiolytic degradation of organic wastes. For methane, 0.32 ppmv corresponds to roughly 0.0006 % of its LFL. Acetonitrile, at 0.0093 ppmv, similarly presents virtually no flammable risk, and is well below its NIOSH 8-hour REL of 20 ppmv.

X.3.2 Tentatively Identified Organic Analytes

In addition to targeted analytes, both ORNL and PNL analytical procedures allow the tentative identification of other organic vapors. By the nature of the samples and their analysis, virtually all 3 to 15 carbon organic compounds present in the tank headspace above analytical detection limits are observable. The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table X-4, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table X-5. Estimated concentrations are in mg/m^3, based on dry air at 0 °C and 1.01 bar.

Both ORNL and PNL tentatively identify analytes 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 also determines its molecular weight (which specifies the number of carbon atoms in the molecule). The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Entries in Table X-5, particularly near the bottoms of the table where the analytes have higher molecular weights, illustrate this.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Lucke et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-4 and X-5 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 22 and 28 in Table X-5). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

Concentrations given in Tables X-4 and X-5 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

X.3.3 Total Nonmethane Organic Compounds

OGIST measured the total nonmethane organic compound (TNMOC) concentration in 3 SUMMA™ canister samples using the EPA TO-12 method (Rasmussen 1994a). The sample mean was 176 $\mu g/m^3$, with a standard deviation of 23 $\mu g/m^3$. Though data on other tanks is very limited, this value is very low compared to other waste

tanks sampled to date. For comparison, the TNMOC concentration in clean ambient air may range from 30 to 100 $\mu g/m^3$, in polluted city air it may be 300 to 400 $\mu g/m^3$, tank C-103 has an estimated 3×10^6 to 5×10^6 $\mu g/m^3$ (Rasmussen and Einfeld 1994), and tank BY-106 has about 9,900 $\mu g/m^3$ (Rasmussen 1994d).

X.3.4 Discussion of Organic Analytes

In general, the organic analytes observed in the waste tank headspaces are indicative of the types of organic waste that have been stored in each tank. Examination of the data provides clues to both the current organic constituents and the chemical reactions that they undergo.

Some of the compounds listed in Tables X-3, X-4, and X-5 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane and n-tridecane) that were used as a diluent for tributyl phosphate in several Hanford processes.

Notably absent from the tank C-111 headspace are the semivolatile cyclic alkanes (e.g., methylated decahydronaphthalenes, cyclopentanes, and cyclohexanes) that have been observed in the 241-BY tank farm. This suggests that, like tank C-103, the semivolatile organic waste in tank C-111 may be from the Plutonium Uranium Extraction (PUREX) process, which in the late 1960's used a relatively pure form of semivolatile NPHs as a process diluent.

Most of the compounds in Tables X-3, X-4, and X-5 are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. For example, 1-butanol is known to be formed by the hydrolysis of tributyl phosphate, and it has been suggested that the alcohols, aldehydes, ketones, nitriles, alkenes, and short chain alkanes are all degradation products of NPHs.

Examination of the compounds listed in Tables X-3, X-4 and X-5 suggests many of the volatile species (presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom. For example, most alcohols are 1-alkanols, and ketones generally have the double bonded oxygen atom on the second carbon atom. In particular, all the normal aldehydes from butanal through dodecanal were detected.

Though their concentrations are not significant, many alcohols and acids were tentatively identified by ORNL (Table X-5). These have generally not been observed to be as numerous in other NPH-rich tank headspaces, which tend to be dominated by aldehydes, ketones, alkanes, and alkenes.

Table X-1
Tank C-111 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	0.5 and 2.0	Organic vapors	8 tank air samples + 2 trip blanks
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous Oxide, Carbon Dioxide, Carbon Monoxide	3 tank air samples
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table X-2
Tank C-111 Inorganic Gas and Vapor Concentrations

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	5.6	0.9	16
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	198	1	0.5
Carbon Monoxide, CO	630-08-0	SUMMA™,[3]	3	0.10	0.01	9
Hydrogen, H_2	1333-74-0	SUMMA™	3	12.4	2	16
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.62	0.05	8
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	6	≤ 0.08	--	--
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	99.3	1.2	1
Water Vapor, H_2O	7732-18-5	Sorbent Trap	6	31,100 (22.2 mg/L)	1,600 (1.1 mg/L)	5

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

3. Carbon monoxide results are from analysis of 9 SUMMA™ samples collected August 10, 1993 (Huckaby 1994a).

Table X-3
Tank C-111 Positively Identified Organic Compound Average Concentrations

Compound	CAS[1] Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
Methane	74-82-8	SUMMA™,[3]	0.32	0.02	5
Ethanenitrile (acetonitrile)	75-05-8	TST[4]	0.0093	0.0019	20
Propanone (acetone)	67-64-1	TST	0.0080	0.0019	24
Dichloromethane[5]	75-09-2	TST	0.18	0.21	116
		SUMMA™	< 0.002	--	--
n-Hexane[5]	110-54-3	TST	0.00044	0.00022	50
Benzene[5]	71-43-2	TST	0.00056	0.00010	18
		SUMMA™	< 0.002	--	--
1-Butanol[5]	71-36-3	TST	0.0016	0.0005	29
Toluene[5]	108-88-3	TST	0.00036	0.00003	8
		SUMMA™	< 0.002	--	--
2-Hexanone[5]	591-78-6	TST	0.00032	0.00007	21
n-Octane[5]	111-65-9	TST	0.000034	0.000056	163
2-Heptanone[5]	110-43-0	TST	0.00032	0.00005	15
n-Nonane[5]	111-84-2	TST	0.000084	0.000071	85
2-Octanone[5]	111-13-7	TST	0.00020	0.00003	14
n-Dodecane[5]	112-70-3	TST	0.00054	0.00005	9
n-Tridecane[5]	629-50-5	TST	0.0012	0.0001	7

Sum of nonmethane positively identified compounds:	0.203

1. CAS = Chemical Abstract Service.

2. RSD = Relative Standard Deviation.

3. SUMMA™ results are based on analyses of 3 samples. Methane results from OGIST, other SUMMA™ results from PNL.

4. TST results are based on analyses of 3 samples.

5. Two or more samples fell outside of calibration range.

Table X-4
Tank C-111 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compounds	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
1	Ethanal (acetaldehyde)	75-07-0	0.093	0.093
2	Propanone (acetone)	110-62-3	0.075	0.075
3	Butanal[2]	123-72-8	0.040	--
4	2-Butanone[2]	78-93-3	0.020	--
5	Pentanal[2]	110-62-3	0.039	--
6	Hexanal[2]	66-25-1	0.049	--
7	Heptanal	111-71-7	0.055	0.005
8	C6-alkene[2]		0.033	--
9	Octanal	124-13-0	0.063	0.008
10	Nonanal	124-19-6	0.066	0.014
11	C7-alkene[2]		0.019	--
12	Decanal[2]	112-31-2	0.023	--
Sum of tentatively identified compounds:			0.58	

1. CAS = Chemical Abstract Service.

2. Detected in only 1 sample.

Table X-5
Tank C-111 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
1	Methane, trichlorofluro	75-69-4	0.035	0.0613
2	Acetic acid	64-19-7	0.038	0.0081
3	Hexanal	66-25-1	0.003	0.0054
4	Cyclotrisiloxane, hexamethyl	541-05-9	0.003	0.0044
5	Heptanal	111-71-7	0.006	0.0022
6	Phenol	108-95-2	0.007	0.0011
7	Cyclotetrasiloxane, octamethyl	556-67-2	0.008	0.0052
8	Octanal	124-13-0	0.010	0.0026
9	1-Hexanol, 2-ethyl	104-76-7	0.009	0.0009
10	1-Octanol	111-87-5	0.001	0.0023
11	Ethanone, 1-phenyl	988-86-2	0.001	0.0023
12	Phenol, 2-methyl	95-48-7	0.001	0.0026
13	Nonanal	124-19-6	0.020	0.0052
14	Benzeneacetic acid, a, 4-bis[(trimethylsilyl	55334-40-2	0.003	0.0027
15	2-Nonenal, (E)	18829-56-6	0.002	0.0038
16	1-Nonanol	143-08-8	0.004	0.0006
17	Decanal	112-31-2	0.011	0.0020
18	Benzothiazole	95-16-9	0.003	0.0005
19	Alkanoic acid and others		0.002	0.0028
20	2(3H)-Furanone, dihydro-5-propyl	105-21-5	0.001	0.0012
21	n-Octan-3-ene		0.001	0.0013
22	Dodecanal	112-54-9	0.003	0.0024
23	5-Nonanone	502-56-7	0.009	0.0009
24	2,5-Pyrrolidinedione, 3-ethyl-3-hydroxy & others		0.007	0.0008
25	2-Nonanone	821-55-6	0.002	0.0032
26	2-Octanol	123-96-6	0.001	0.0012

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
27	Phthalate		0.001	0.0014
28	Dodecanal	112-54-9	0.001	0.0011
29	5,9-Undecadien-2-one, 6,10-dimethyl-(Z)	3879-26-3	0.001	0.0023
30	Undecanal	112-44-7	0.002	0.0021
31	Benzenamine,n-phenyl & others	103-32-2	0.001	0.0026
32	Decane, 1,1'-oxybis-	2456-28-2	0.008	0.0025
33	9H-fluorene.3-methyl & di-t-butyl-ethylphe		0.004	0.0019
34	2,5-cyclohexadiene-1,4-dione, 2,6-bis(1,1	719-22-2	0.003	0.0017
35	Alkanol		0.001	0.0018
36	2-Decanone	693-54-9	0.001	0.0013
37	2-Dodecanone	6175-49-1	0.002	0.0019
38	Decanoic acid	334-48-5	0.001	0.0016
39	Hexadecanoic acid	57-10-3	0.001	0.0020
40	1,2-Benzenedicarboxylic acid, diethyl ester	84-66-2	0.009	0.0014
41	Benzenamine, n-phenyl	122-39-4	0.008	0.0017
42	1-Hexanol, 2-ethyl	104-76-7	0.001	0.0011
43	Tetradecanoic acid	544-63-8	0.013	0.0046
44	Alkane		0.004	0.0036
45	Decane, 4-cyclohexyl-, 4-cyclohexyl	13151-75-2	0.001	0.0012
46	Alkane		0.002	0.0036
47	9-Octadecanoic acid, (Z)-	112-80-1	0.001	0.0015
48	Pentadecanoic acid	1002-84-2	0.006	0.0032
49	1-Octadecene	112-88-9	0.001	0.0011
50	9-Octadecenen-1-ol, (Z)	143-28-2	0.002	0.0031
51	9-Hexadecenoic acid	2091-29-4	0.010	0.0095

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
52	Hexadecanoic acid	57-10-3	0.041	0.0159
53	Eicosane	112-95-8	0.005	0.0049
54	1-Hexadecanol	36653-82-4	0.001	0.0025
55	16-Methylheptadecanol-1		0.001	0.0025
Sum of tentatively identified compounds:			0.33	

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