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Tank 241-C-112 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-426)		ECN No. 623549

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ENGINEERING CHANGE NOTICE

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1. ECN No 623549

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
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[] 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): 623549

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	
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Other		Other	
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RELEASE AUTHORIZATION

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

APPROVED FOR PUBLIC RELEASE

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SUPPORTING DOCUMENT

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241-C-112, 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-112 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-112 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).

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RECORD OF REVISION	(1) Document Number WHC-SD-WM-ER-426	Page 1

(2) Title
Tank 241-C-112 Vapor Sampling and Analysis Tank Characterization Report

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release	
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Tank 241-C-112 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank C-112 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-112 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-112.

X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank C-112 using the vapor sampling system (VSS) on August 11, 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 28 °C. Air from the tank C-112 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 4, 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 and 2 field 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

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

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 (Ligotke 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 about 1 % for carbon monoxide results, to 8 % for nitric oxide 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, 22.7 ppmv, is close to the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995). Ammonia concentrations have been observed to be higher than this level in the waste tank headspaces. The relatively low ammonia concentration in tank C-112 may be related to the fact that only a small quantity of relatively cool waste is stored in tank C-112.

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 204 ppmv of hydrogen in tank C-112, however, represents only about 0.5 % 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-112, 544 ppmv, is about 22 times the NIOSH 8-hr REL of 25 ppmv (NIOSH 1995).

For comparison, the measured concentrations of ammonia, hydrogen, and nitrous oxide for the 4 Ferrocyanide Watchlist waste tanks in 241-C farm are given in Table X-3. The waste in these tanks is principally sludge. As indicated in Table X-3, in each of these 4 tanks the nitrous oxide concentration is higher than the hydrogen concentration, which in turn is higher than the ammonia concentration. Of these tanks, tank C-112 has the highest concentrations of ammonia, hydrogen, and nitrous oxide.

X.2.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 102 ppmv, is one-fourth 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 liquid, and condensate) in the tank. Carbon dioxide concentrations in the other Ferrocyanide Watchlist tanks in 241-C farm are given in Table X-3 for comparison.

Carbon monoxide in the tank C-112 headspace, at about 0.92 ppmv, is above its concentration in 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.

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

Nitric oxide and nitrogen dioxide concentrations in the tank C-112 headspace were determined to be 0.62 ppmv and $\leq$ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-112. 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-112 was determined to be about 22.3 mg/L, at the tank headspace temperature of 28 °C and pressure of 989 mbar (742 torr), (WHC 1995). This corresponds to water vapor partial pressure of 31.0 mbar (23.2 torr), to a dew point of 24.6 °C, and to a relative humidity of 82 %. The water vapor content of the tank C-112 headspace is typical of other 241-C farm tanks.

Silica gel sorbent traps were used to test for tritium. It is assumed that tritium produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Analysis of the silica gel, which would have trapped approximately 26 mg of water vapor, indicated the total activity of the sample to be below the method detection limit of 50 pCi (WHC 1995).

X.3 ORGANIC VAPORS

Organic vapors in the tank C-112 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 Ligotke 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-112. 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 22 of 27 target analytes selected by WHC, (5 analytes were below detection limits). These analytes, and their average concentrations from the analysis of 4 TSTs, are given in Table X-4. The 27 TST target analytes for tank C-112 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 22 analytes positively identified by ORNL, only propanenitrile and 1-butanol were within the calibration range of the method. Two of the target analytes were detected above the calibration range, and 18 were detected below the calibration range. These concentrations are known with much greater certainty than the concentrations of tentatively identified compounds in Table X-6, but are not technically quantitative.

Also given in Table X-4 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, Ligotke et al. 1995). Except for about 0.0035 ppmv of toluene detected in 1 SUMMA™ canister sample, none of the 40 TO-14 analytes were observed to be above the 0.002 ppmv quantitation limit of the analyses (Ligotke 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. ORNL detected trace amounts of dichloromethane and benzene, but these were both below the limit of detection of PNL (0.002 ppbv). The 0.0035 ppmv of toluene detected in a single PNL sample is not supported by the ORNL analyses.

The 2 most abundant analytes in Table X-4 are methane and acetonitrile. At 1.013 ppmv, the methane concentration in tank C-112 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, 1.0 ppmv corresponds to roughly 0.002 % of its LFL. Acetonitrile, at 3.0 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-5, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table X-6. 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-6, particularly near the bottom 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 Ligotke et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-5 and X-6 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 70 and 76 in Table X-6). 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-5 and X-6 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 3,360 $\mu g/m^3$, with a standard deviation of 100 $\mu g/m^3$. Though data on other tanks is very limited, this value is about average 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 1994b).

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-4, X-5, and X-6 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, n-tridecane, n-tetradecane, n-pentadecane) that were used as a diluent for tributyl phosphate.

Notably absent from the tank C-112 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-112 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-4, X-5, and X-6 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-4, X-5 and X-6 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.

Though their concentrations are not significant, many alcohols and acids were tentatively identified by ORNL (Table X-6). 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-112 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	1.0 and 4.0	Organic vapors	8 tank air samples + 2 trip blanks + 2 field 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-112 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	22.7	0.5	2
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	102	1	1
Carbon Monoxide, CO	630-08-0	SUMMA™	3	0.92	0.02	3
Hydrogen, H_2	1333-74-0	SUMMA™	3	204	5	3
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.62	0.05	8
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	544	9	2
Water Vapor, H_2O	7732-18-5	Sorbent Trap	6	31,300 (22.3 mg/L)	1,800 (1.3 mg/L)	6

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

Table X-3
Comparison of Selected Analytes
in Ferrocyanide Watchlist 241-C Farm Tanks

Tank	Ammonia (ppmv)	Hydrogen (ppmv)	Nitrous Oxide (ppmv)	Carbon Dioxide (ppmv)
241-C-108[1]	2.7	15.3	344	16.3
241-C-109[2]	10.1	125	369	3
241-C-111[3]	5.6	12.4	99.3	198
241-C-112	22.7	204	544	102
Average:	10.3	89	339	80

1. Ammonia results are from Lucke et al. 1995a, other analytes are from Rasmussen 1994c.

2. Ammonia results are from Pool et al. 1995, other results are from Rasmussen 1994d.

3. Ammonia results are from Lucke et al. 1995b, other results are from Rasmussen 1994e.

Table X-4
Tank C-112 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]	1.013	0.006	0.6
Ethaneitrile[4] (acetonitrile)	75-05-8	TST[5]	3.0	0.9	31
Propanone[4] (acetone)	67-64-1	TST	0.078	0.018	23
Dichloromethane[6,7] (methylene chloride)	75-09-2	TST	0.00018	--	--
		SUMMA™	< 0.002	--	--
Propanenitrile	107-12-0	TST	0.023	0.006	26
n-Hexane[7,8]	110-54-3	TST	0.00009	0.00001	13
Benzene[7,8]	71-43-2	TST	0.00011	0.00002	22
		SUMMA™	< 0.002	--	--
1-Butanol	71-36-3	TST	0.0044	0.0017	39
Butanenitrile[7]	109-74-0	TST	0.0032	0.0007	23
2-Pentanone[7]	107-87-9	TST	0.0012	0.0005	43
n-Heptane[7]	142-82-5	TST	0.00071	0.00054	77
Toluene[6]	108-88-3	TST	<0.0003	--	--
		SUMMA™	0.0035	--	--
Pentanenitrile[7]	110-59-8	TST	0.00037	0.00006	15
2-Hexanone[7]	591-78-6	TST	0.00031	0.00008	27
n-Octane[7]	111-65-9	TST	0.00016	0.00007	46
Hexanenitrile[7,9]	628-73-9	TST	0.00017	0.00002	9

Compound	CAS[1] Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
2-Heptanone[7]	110-43-0	TST	0.00021	0.00005	22
n-Nonane[7]	111-84-2	TST	0.00012	0.00005	45
Heptanenitrile[7,9]	629-08-3	TST	0.00015	0.00002	14
2-Octanone[7,9]	111-13-7	TST	0.00010	0.00001	11
Octanenitrile[7,9]	124-12-9	TST	0.000063	0.000014	21
Nonanenitrile[7,9]	2243-27-8	TST	0.000087	0.000013	15
n-Dodecane[7]	112-40-3	TST	0.00043	0.00008	19
n-Tridecane[7]	629-50-5	TST	0.00060	0.00007	11
Sum of nonmethane positively identified compounds:			5.7 mg/m^3		

1. CAS = Chemical Abstract Service.

2. RSD = Relative Standard Deviation.

3. SUMMA™ results are based on analyses of 3 samples. Methane results are from Rasmussen 1994a, other SUMMA™ results are from Ligotke et al. 1995.

4. Results are above upper calibration limit.

5. TST results are based on analyses of 4 samples, except where noted.

6. Detected in only 1 sample.

7. Results are below lower calibration limit.

8. Detected in only 2 samples.

9. Detected in only 3 samples.

Table X-5
Tank C-112 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviations (mg/m^3)
1	Ethanal (acetaldehyde)	75-07-0	0.17	0.09
2	Ethanenitrile (acetonitrile)	75-05-8	1.99	0.09
3	Propanone (acetone)	67-64-1	0.56	0.01
4	Methyl Nitrate	598-58-3	0.20	0.01
5	Propanenitrile	107-12-0	0.07	0.05
Sum of tentatively identified compounds:			2.99	

1. CAS = Chemical Abstract Service.

Table X-6
Tank C-112 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
1	Trichlorofluoromethane	75-69-4	0.001	0.002
2	Nitric acid, methyl ester		0.030	0.009
3	Nitric acid, ethyl ester	625-58-1	0.003	0.003
4	Propanenitrile, 2,2-dimethyl	630-18-2	0.002	0.003
5	Acetic acid	64-19-7	0.003	0.003
6	2-Butanone, 3,3-dimethyl	75-97-8	0.001	0.001
7	Siloxane and others		0.001	0.001
8	Nitric acid, propyl ester		0.002	0.002
9	Cyclopropanecarbonnitrile	5500-21-0	0.006	0.005
10	Propane, 2-methyl-2-nitro	594-70-7	0.010	0.007
11	Alkanol		0.001	0.002
12	Nitric acid, ester		0.001	0.001
13	Siloxane and others		0.006	0.005
14	Hexanal	66-25-1	0.001	0.002
15	2H-Pyran-2-one, tetrahydro-5,6-dimethyl	22405-16-1	0.005	0.011
16	1-Propanol, 2,2-dimethyl, nitrate	926-42-1	0.001	0.001
17	Cyclotrisiloxane, hexamethyl	541-05-9	0.009	0.009
18	Heptanal	111-71-7	0.001	0.001
19	2-Heptanone, 3-methyl	2371-19-9	0.002	0.002
20	Oxirane, ethenyl	930-22-3	0.018	0.005
21	2-Heptanone, 6-methyl	928-68-7	0.001	0.001
22	Cyclotetrasiloxane, octamethyl	556-67-2	0.005	0.003
23	2-Heptanone, 4-methyl and others	110-43-0	0.002	0.001
24	Octanal	124-13-0	0.001	0.002
25	2H-Pyran-2-one, tetrahydro-6,6-dimethyl	2610-95-9	0.002	0.001
26	1-Hexanol,2-ethyl	104-76-7	0.0005	0.001
27	Isothiazole	288-16-4	0.001	0.001

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
28	Ethanone, 1-phenyl	98-86-2	0.004	0.003
29	Benzenemethanol, a,a,-dimethyl	617-94-7	0.001	0.001
30	Nonanal	124-19-6	0.004	0.002
31	1-Decene and others	124-19-6	0.001	0.001
32	Decanal	112-31-2	0.003	0.002
33	Undecane, 3,6-dimethyl	17301-28-9	0.001	0.001
34	Decane, 2,2,6-trimethyl	62237-97-2	0.001	0.001
35	C13-Alkane		0.001	0.001
36	Alkane		0.0003	0.001
37	1-Hexanol, 2-ethyl	104-76-7	0.0004	0.001
38	1H-Azepin-1-amine,N-ethylidenehexahydro	75268-01-8	0.008	0.002
39	Alkane and others		0.001	0.003
40	Heptane, 2,2,4,6,6-pentamethyl	13475-82-6	0.006	0.001
41	C13-Alkane		0.002	0.001
42	Nonane, 3-methyl-5-propyl	31081-18-2	0.002	0.002
43	C13-Alkane		0.002	0.001
44	C13-Alkane		0.001	0.001
45	Mixture		0.0003	0.001
46	Decane, 2,6,8-trimethyl	62108-26-3	0.001	0.001
47	Alkane		0.0003	0.001
48	Undecane, 3,5-dimethyl	17312-81-1	0.0003	0.001
49	Alkane		0.0003	0.001
50	C13-Alkane		0.002	0.001
51	Propanoic acid, 2-methyl-3-hydroxy-2,4,4-	74367-34-3	0.0004	0.001
52	C6 ester of butanoic acid		0.0004	0.001
53	Tetradecane	629-59-4	0.005	0.000
54	C15-Alkane		0.002	0.001
55	1-Hexadecanol	29354-98-1	0.0003	0.001

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
56	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1	719-22-2	0.0003	0.001
57	Pentadecane	629-62-9	0.002	0.001
58	Dodecanoic acid	143-07-7	0.004	0.002
59	C16-alkane		0.0005	0.001
60	Heptadecane	629-78-7	0.0004	0.001
61	Propanoic acid, 2-methyl-,1-(1,1-dimethyle	74381-40-1	0.037	0.014
62	Alkane		0.002	0.005
63	Benzenamine, N-phenyl	122-39-4	0.005	0.003
64	Alkane		0.001	0.002
65	Benzenesulfonamide, N-alkyl	98-10-2	0.001	0.002
66	Phenoxy Benzaldehyde		0.001	0.001
67	Nonadecane	629-92-5	0.0004	0.001
68	1-Hexadecanol	36653-82-4	0.0003	0.001
69	1,1'-Biphenyl,2,2'-diethyl	13049-35-9	0.001	0.001
70	Tetradecanoic acid	544-63-8	0.020	0.008
71	Alkanoic acid and others		0.001	0.003
72	Alkanoic acid and others		0.001	0.003
73	Hexanedioc acid, dioctyl ester	123-79-5	0.004	0.008
74	Benzenesulfonamide, N-butyl	3622-84-2	0.081	0.042
75	Alkane		0.000	0.001
76	Tetradecanoic acid	544-63-8	0.024	0.036
77	2-Octadecenal	56554-96-2	0.0003	0.001
78	Alkane		0.002	0.002
79	9-Headecenoic acid	2091-29-4	0.006	0.007
80	Cyclohexanecarboxylic acid, 2-(1,1-dimeth	27392-16-1	0.001	0.001
81	Alkene		0.005	0.007

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
82	Hexadecanoic acid	57-10-3	0.035	0.013
83	Phthalate		0.001	0.001
84	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.001	0.001
85	Alkane		0.001	0.001
86	10-dimethylsqualene		0.003	0.006
Sum of tentatively identified compounds:			0.41	

1. CAS = Chemical Abstract Service.

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