DISTRIBUTION SHEET

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Project Title/Work Order		EDT No.
Tank 241-BY-104 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-418)		ECN No. 623541

Name	MSIN	Text With All Attach.	Text Only	Attach./ Appendix Only	EDT/ECN Only
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COMPLETE

ENGINEERING CHANGE NOTICE

Page 1 of 2

1. ECN No 623541

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. Vapor Sampling	6. Bldg./Sys./Fac. No. 200 Gen	7. Approval Designator N/A
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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 cnaveat 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)

See attached distribution sheet

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DATE MAY 31 1995

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1. ECN (use no. from pg. 1): 623541

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-418, REV 1
Document Title:	Tank 241-BY-104 Vapor Sampling and Analysis Tank Characterization Report
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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 25

2. Title	3. Number	4. Rev No.
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5. Key Words	6. Author
241-BY-104, 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-BY-104 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-BY-104 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-418	Page 1

(2) Title

Tank 241-BY-104 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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RS 1	(7) Made editorial changes and added information in organic vapor chapter.	J.W. Osborne	T. Kelley 5-31-95
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Tank 241-BY-104 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank BY-104 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 BY-104 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

X.1 SAMPLING EVENT

Headspace vapor samples were collected from tank BY-104 using the vapor sampling system (VSS) on June 24, 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). Tank BY-104 was the first tank to be vapor sampled after the effectiveness of the VSS had been demonstrated on tank C-103. Air from the tank BY-104 headspace was withdrawn via a heated sampling probe mounted in riser 10A, and transferred via heated tubing to the VSS sampling manifold.

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. The 46 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 10 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.

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), except for water vapor, which is given in mg/L. Sorbent traps were prepared and analyzed by PNL, SUMMA™ canisters were

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

analyzed by OGIST. Reports by Clauss et al. (1994) and Rasmussen (1994) 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 very good. Relative standard deviations range from 2 % for ammonia results to 14 % 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, 248 ppmv, is about 10 times higher than the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995), and greater than the average tank headspace ammonia concentrations measured to date. Ammonia concentrations at this level are not uncommon in the waste tank headspaces, and are known to as high as about 1040 ppmv in tank BY-108 (McVeety et al. 1995).

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 295 ppmv of hydrogen in tank BY-104, however, represents only about 0.7 % 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 BY-104, 201 ppmv, is about 8 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, 10.5 ppmv, is markedly lower than normal ambient air concentrations of about 400 ppmv. Little data on waste tank headspace carbon dioxide concentrations is available, but lower than ambient 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. The very low carbon dioxide level in tank BY-104 may be a symptom of the manner in which the headspace breathes with the atmosphere (i.e., air inflow may come from tank BY-105), or some characteristic of the waste itself.

Carbon monoxide in the tank BY-104 headspace, at about 1.0 ppmv, is more concentrated than in ambient air, where it typically is about 0.05 to 0.15 ppmv. Carbon monoxide may be a decomposition of organic waste in tank BY-104. With a NIOSH 8-hr REL of 35 ppmv (NIOSH 1995), the 1.0 ppmv in tank BY-104 probably does not represent a worker hazard.

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

Nitric oxide and nitrogen dioxide concentrations in the tank BY-104 headspace were determined to be 0.29 ppmv and ≤ 0.07 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH interstitial liquid in tank BY-104. 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 BY-104 was determined to be about 14.1 mg/L, at the measured tank headspace temperature of 26 °C and pressure of 994 mbar (747 torr), (WHC 1995). This corresponds to water vapor partial pressure of 19.4 mbar (14.6 torr), to a dew point of 17.0 °C, and to a relative humidity of 58 %.

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, which would have trapped approximately 32 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 BY-104 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 Clauss et al. (1994). 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 1994).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-104. 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 and quantitated 26 of 27 analytes selected by WHC, (1 analyte, vinylidene chloride was below detection limits). These analytes, arranged in the approximate order of chromatographic elution, are given in Table X-3. Also given in Table X-3 are the analytes' average concentrations from the analysis of 4 TSTs. The TST target analytes for tank BY-104 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).

Also given in Table X-3 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL. PNL performed analyses according to the EPA TO-14 methodology (EPA 1988, Lucke et al. 1994). Only 4 of the 40 TO-14 analytes were observed to be above the general 0.002 ppmv quantitation limit of the analyses (Clauss et al. 1994 provide the complete TO-14 analyte list). Averages reported are from analyses of 3 SUMMA™ canister samples except where noted.

Three analytes in Table X-3 were common to both the ORNL and PNL analyses: dichloromethane, benzene, and toluene. The ORNL and PNL results agree for dichloromethane, but differ by more than a factor of 4 for toluene, and by more than a factor of 12 for benzene. Though these differences are greater than the allowed ±30 % analytical accuracy, they are not unreasonable given that fundamentally different sampling devices and analytical methods were used. What is important in this case is that both ORNL and PNL benzene results, 0.042 ppmv and 0.0031 ppmv respectively, are well below its NIOSH REL of 1 ppmv. Similarly, the ORNL and PNL toluene results, 0.41 ppmv and 0.010 ppmv respectively, are well below its NIOSH REL of 100 ppmv.

The 3 most abundant organic compounds in the tank BY-104 headspace are methane, acetone, and 1-butanol. At 8.2 ppmv, the methane concentration is about 4 times higher than its normal ambient air concentration. Methane is probably formed during the chemical and radiolytic degradation of organic wastes in tank BY-104. Methane is not a constituent of toxicological concern, and its LFL in air is about 5 % by volume. This places the 8.2 ppmv of methane in tank BY-104 at less than 0.02 % of its LFL. Acetone, at 1.2 ppmv, and 1-butanol, at 1.0 ppmv, are the only other organic constituents at or above the 1 ppmv level.

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. Table X-4 is a reproduction of the PNL list of tentatively identified compounds, with estimated concentrations, and Table X-5 is a reproduction of the ORNL list of tentatively identified compounds, and their estimated concentrations in mg/m^3, in 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 Tables X-4 and X-5, particularly near the bottoms of the tables where the analytes have higher molecular weights, illustrate this.

The PNL and ORNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1994), 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 chromatographically split peaks (e.g., Cmpd # 3 and 4, 24 and 28 in Table X-5). In these instances, the estimated concentration of a compound identified in different peaks 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 1994). The sample mean was 60,800 $\mu g/m^3$, with a standard deviation of 5,900 $\mu g/m^3$. Though data on other tanks is very limited, this value is relatively high, and suggests that tank BY-104 has relatively large inventory of volatile and semivolatile organic waste.

X.3.4 Discussion of Organic Analytes

The organic analytes observed in the waste tank headspaces are indicative of the types of semivolatile 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 tributyl phosphate, which was used as an extractant in several Hanford processes; dibutyl butylphosphonate, which was a contaminant of tributyl phosphate; and the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-undecane, n-dodecane, n-tridecane, and n-pentadecane) and branched and cyclic alkanes (e.g., methylated decahydronaphthalenes,

cyclopentanes, and cyclohexanes) with similar boiling points that were used as a diluent for tributyl phosphate.

Most of the compounds in Tables X-3, X-4, and X-5, however, are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. Specifically, 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 alkenes listed have their double bond between the first and second carbon atoms, and ketones generally have the double bonded oxygen atom on the second carbon atom.

As observed in other NPH-containing waste tanks, there are many small cyclic compounds, specifically cyclopropanes, cyclopentanes, and furans. The presence of these suggest that organic radicals, formed in the radiation field of the tank, play a role in the degradation of the semivolatile compounds.

Table X-1
Tank BY-104 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	2.0	Organic vapors	4 tank air samples + 2 trip blanks
Oregon Graduate Institute of Science and Technology	SUMMA™ canister	6.0	Hydrogen, Nitrous oxide, Carbon dioxide, Carbon monoxide, Organic vapors	3 tank air samples
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	5 tank air samples + 2 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen dioxide	10 tank air samples + 2 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric oxide	10 tank air samples + 2 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	10 tank air samples + 2 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	2.0	Tritium-substituted water vapor	1 tank air sample

Table X-2
Tank BY-104 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	5	248	5	2
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	10.5	0.7	7
Carbon Monoxide, CO	630-08-0	SUMMA™	3	1.0	0.11	11
Hydrogen, H_2	1333-74-0	SUMMA™	3	295	15	5
Nitric Oxide, NO	10102-43-9	Sorbent Trap	10	0.29	0.04	14
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	10	≤ 0.07	--	--
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	201	8	4
Water Vapor, H_2O	7732-18-5	Sorbent Trap	10	19,500 (14.1 mg/L)	1,100 (0.8 mg/L)	6

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

Table X-3
Tank BY-104 Positively Identified Organic Compound Average Concentrations

Compound	CAS[1] Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
Methane[3]	74-82-8	SUMMA™,[4]	8.2	0.3	4
Dichlorodifluoromethane	75-71-8	SUMMA™	0.0008	0.0002	19
Chloromethane (Methyl chloride)	74-87-3	SUMMA™	0.0017[5]	--	--
Trichlorofluoromethane	75-69-4	SUMMA™	0.360	0.046	13
Dichloromethane (Methylene chloride)	75-09-2	TST[6]	0.002	0.0004	20
		SUMMA™	0.0018[5]	--	--
Ethanenitrile (Acetonitrile)	75-05-8	TST	0.33	0.086	26
Propanone (Acetone)	67-64-1	TST	1.2	0.293	24
Propanenitrile	107-12-0	TST	0.016	0.003	21
Butanal	123-72-8	TST	0.16	0.038	24
n-Hexane	110-54-3	TST	0.32	0.027	9
Benzene	71-43-2	TST	0.042	0.011	27
		SUMMA™	0.0031	0.0007	22
1-Butanol	71-36-3	TST	1.0	0.090	9
Butanenitrile	109-74-0	TST	0.020	0.002	11
2-Pentanone	107-87-9	TST	0.16	0.016	10
n-Heptane	142-82-5	TST	0.12	0.011	9
Toluene	108-88-3	TST	0.041	0.012	30
		SUMMA™	0.010	0.003	24
Tetrachloroethene	127-18-4	SUMMA™	0.0016[3]	--	--
Ethylbenzene	100-41-4	SUMMA™	0.0018	0.0001	5

Compound	CAS[1] Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
1,3-Dimethylbenzene (m-xylene) + 1,4-Dimethylbenzene (p-xylene)	108-38-3 106-42-3	SUMMA™	0.0048	0.0002	4
1,2-Dimethylbenzene (o-xylene)	95-47-6	SUMMA™	0.0017	0.0001	8
Pentanenitrile	110-59-8	TST	0.012	0.002	19
2-Hexanone	591-78-6	TST	0.065	0.010	16
n-Octane	111-65-9	TST	0.059	0.006	11
Hexanenitrile	628-73-9	TST	0.010	0.001	12
2-Heptanone	110-43-0	TST	0.048	0.005	11
n-Nonane	111-84-2	TST	0.028	0.001	5
Heptanenitrile	629-08-3	TST	0.007	0.0007	11
2-Octanone	111-13-7	TST	0.015	0.002	11
Octanenitrile	124-12-9	TST	0.003	0.0002	8
Nonanenitrile	2243-27-8	TST	0.002	0.0004	16
n-Dodecane	112-40-3	TST	0.058	0.003	6
n-Tridecane	629-50-5	TST	0.084	0.008	10
Tributyl phosphate (TBP)	126-73-8	TST	0.00082	0.00009	
Dibutyl butylphosphonate (DBBP)	75-46-4	TST	0.000087	0.00001	

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. Methane results are from Rasmussen 1994.

4. All SUMMA canister results are based on analyses of 3 samples.

5. Result from only 1 sample, < 0.002 ppmv in other samples.

6. Except where noted, all TST results are based on 4 samples.

Table X-4
Tank BY-104 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
1	Propene	115-07-1	1.35	0.66
2	Propane	74-98-6	0.60	0.28
3	Cyclopropane	75-19-4	0.17	0.08
4	2-Methylpropane	75-28-5	0.35	0.17
5	2-Butene	107-01-7	0.65	0.33
6	n-Butane	106-97-8	0.76	0.37
7	2-Methylpropene	115-11-7	0.15	0.08
8	2-Methyl-2-Butene[3]	513-35-9	0.05	0.09
9	Propanone (acetone)	67-64-1	1.99	1.01
10	1-Pentene	109-67-1	0.30	0.19
11	n-Pentane	109-66-0	0.79	0.57
12	4-Methyl-1-pentene[3]	691-37-2	0.05	0.09
13	2-Methylpentane	107-83-5	1.03	0.22
14	Butanal	123-72-8	0.16	0.03
15	Butanone	78-93-3	0.51	0.11
16	3-Methylpentane	96-14-0	0.23	0.02
17	1-Hexene	107-01-7	0.23	0.03
18	n-Hexane	110-54-3	0.79	0.19
19	Tetrahydrofuran	109-99-9	0.20	0.04
20	Methylcyclopentane	96-37-7	0.11	0.01
21	1-Butanol	71-36-3	0.68	0.15
22	2-Pentanone	107-87-9	0.45	0.19
23	3-Methylhexane	589-34-4	0.35	0.06
24	Heptene		0.11	0.03
25	n-Heptane	142-82-5	0.53	0.10
26	C_6 Ketone[3]		0.03	0.05
27	Methylcyclohexane	108-87-2	0.10	0.01
28	2-Methylheptane	592-27-8	0.20	0.03
29	2-Hexanone	591-78-6	0.18	0.03
30	n-Octane	111-65-9	0.22	0.03
31	C_9 Alkane		0.09	0.01

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)	Standard Deviation (mg/m^3)
32	1-Heptanol[4]	111-70-6	0.10	0.02
33	Trimethylcyclohexane[4]		--	--
34	3-Heptanone	106-35-4	0.17	0.02
35	2-Heptanone	110-43-0	0.16	0.03
36	2-Butoxyethanol	111-76-2	0.10	0.02
37	n-Nonane	111-84-2	0.14	0.02
38	6-Methylheptanone		0.31	0.05
39	2-Octanone	111-13-7	0.05	0.05
40	n-Decane	124-18-5	0.14	0.03
41	C_{11} Alkane		0.03[2]	0.05
42	n-Undecane	1120-21-4	0.37	0.08
43	Methyldecahydronaphthalene		0.09	0.02
44	C_5 Cyclohexane		0.13	0.02
45	C_{10} Alkane		0.14	0.03
46	Methyldecahydronaphthalene		0.17	0.02
47	C_{12} Alkane		0.12	0.02
48	n-Dodecane	112-70-3	1.58	0.37
49	C_{12} Alkane		0.14	0.27
50	Alkane		0.64	0.12
51	C_{13} Alkane		0.15	0.30
52	n-Tridecane	629-50-5	0.22	0.52
53	C_{14} Alkane		0.12	0.20
54	n-Tetradecane	629-59-4	0.13	0.22
55	C_{15} Alkane		0.04	0.05
56	n-Pentadecane	629-62-9	0.02	0.02

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero.

3. Detected in only 1 sample, average includes zeros of other samples.

4. Compound #32 and #33 were coelutents, concentration given for #32 is that of their sum.

Table X-5
Tank BY-104 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
1	1-Butene	106-98-9	0.66
2	Butane	106-97-8	0.73
3	1-Propene, 2-methyl	115-11-7	0.12
4	1-Propene, 2-methyl	115-11-7	0.26
5	2-Butene	107-01-7	0.09
6	1-Butene, 3-methyl	563-45-1	0.08
7	Butane, 2-methyl	78-78-4	0.90
8	2-Propanol and others	67-63-0	0.14
9	Methane, trichlorofluoro	75-69-4	0.58
10	Cyclopropane, ethyl	1191-96-4	0.76
11	C5-Alkane		1.02
12	Mixture of pentene and pentyne		0.29
13	2-Propanol	67-63-0	0.14
14	2-Pentene, (Z)	627-20-3	0.09
15	Cyclopentane	287-92-3	0.16
16	Cyclopropane, 1,1-dimethyl	1630-94-0	0.09
17	1,3-Butadiene, 2-methyl	78-79-5	0.12
18	Mixture of 2-propanenitrile & C6-Alkane		0.10
19	1,3-Butadiene, 2-methyl	78-79-5	0.04
20	1-Pentene, 4-methyl	691-37-2	0.36
21	Cyclobutanone	1191-95-3	0.15
22	Pentane, 2-methyl	107-83-5	1.95
23	C6-Alkene		0.36
24	1-Hexene	592-41-6	0.02
25	C6-Alkene		0.01
26	Pentane, 3-methyl	96-14-0	0.48
27	1-Pentene, 2-methyl	763-29-1	0.22
28	1-Hexene	592-41-6	0.49
29	3-Buten-2-one	78-94-4	0.16
30	2-Butanone	78-93-3	1.39
31	Furan, 2-methyl-	534-22-5	0.02

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
32	2-Hexene, (E)	4050-45-7	0.09
33	2-Butene, 2,3-dimethyl	563-79-1	0.12
34	2-Butanol and others	15892-23-6	0.03
35	2-Propanol	67-63-0	0.06
36	Cyclopropane, propyl	2415-72-7	0.11
37	Mixture		0.11
38	Cyclopropane, (1-methylethyl)-	3638-35-5	0.29
39	2-Propanol	67-63-0	0.46
40	Propanenitrile, 2-methyl	78-82-0	0.02
41	Tetrahydrofuran	109-99-9	0.79
42	1,3-Pentadiene,2-methyl	1118-58-7	0.25
43	1,4-Hexadiene	592-45-0	0.14
44	2-Butanol, 2-methyl	75-85-4	0.04
45	1,4-Hexadiene and siloxane	592-45-0	0.02
46	C7-Alkene		0.04
47	1,5-Hexadiene	592-42-7	0.12
48	Cyclohexane	110-82-7	0.05
49	Pentanal	110-62-3	0.02
50	2-Butanone, 3-methyl	563-80-4	0.05
51	Hexane, 2-methyl	591-76-4	0.17
52	C8-Alkene		0.02
53	Formic acid, butyl ester		0.01
54	1,4-Hexadiene	592-45-0	0.01
55	3-Buten-2-one, 3-methyl	814-78-8	0.02
56	2-Propenal,2-methyl	78-85-3	0.05
57	Cyclopentane, 1,2-dimethyl	2452-99-5	0.05
58	3-Heptene, (E)	14686-14-7	0.02
59	Alkanol		0.03
60	2-Heptene	592-77-8	0.05
61	2,3-Pentanedione	600-14-6	0.02
62	Furan, 2,5-dimethyl	625-86-5	0.01
63	3-Pentanone, 2-methyl	565-69-5	0.05
64	2-Heptene (E)	592-77-8	0.03

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
65	Cyclohexane, methyl	108-87-2	0.17
66	Nitric Acid, ethyl ester	625-58-1	0.00
67	Unknown		0.02
68	Alkene and others		0.03
69	Alkane and others		0.01
70	Cyclopentane, ethyl	1640-89-7	0.01
71	2-Pentanol, 2-methyl	590-36-3	0.05
72	Cyclopentane, 1,2,4-trimethyl-,(1.alpha,	4850-28-6	0.02
73	Pentanal, 2-methyl	123-15-9	0.23
74	Siloxane and others		0.04
75	3-Pentanone, 2-methyl	565-69-5	0.01
76	2-Pentanone, 3-methyl	565-61-7	0.03
77	Unknown		0.01
78	Butane, 2,2,3,3-tetramethyl	594-82-1	0.02
79	1-Pentene, 3,4-dimethyl	7385-78-6	0.06
80	Alkane and siloxane		0.06
81	Heptane, 2-methyl	592-27-8	0.15
82	4-Pentenal, 2-ethyl		0.02
83	C8-Alkane		0.08
84	Heptane, 4-methyl	589-53-7	0.12
85	Alkene		0.32
86	Alkanol		0.02
87	1,4-Hexadiene, 4-methyl	1116-90-1	0.01
88	2-Hexanone, 5-methyl	110-12-3	0.04
89	3-Hexanone	589-38-8	0.14
90	C7-Alkene		0.01
91	2-Ethyl-5-methylfuran	1703-52-2	0.01
92	Alkanol		0.01
93	2-Hexanal		0.01
94	3-Octene, (E)	14919-01-8	0.13
95	Tetrachloroethylene	127-18-4	0.01
96	Acetic acid, butyl ester	123-86-4	0.02
97	Hexamethylcyclotrisiloxane	541-05-9	0.01

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
98	Pyridine, 4-methyl	108-89-4	0.00
99	2-Hexenal	505-57-7	0.01
100	Mixture		0.01
101	Heptane, 2,6-dimethyl	1072-05-5	0.13
102	Phenol, 2-methyl	95-48-7	0.01
103	3-Penten-1-ol and others		0.02
104	Cyclohexane, ethyl	1678-91-7	0.04
105	C7-Alkanone		0.01
106	Cyclohexane, 1,1,3-trimethyl	3073-66-3	0.06
107	Mixture		0.09
108	Mixture		0.08
109	2-Hexanone, 4-methyl	105-42-0	0.14
110	C7-Alkanone		0.05
111	Cycloheexane,1,3,5-trimethyl,(1-alpha,3-m	1795-27-3	0.01
112	Heptane, 2,3-dimethyl	3074-71-3	0.04
113	Heptane, 2,6-dimethyl	1073-05-5	0.04
114	C9-Alkane		0.17
115	Benzene, 1,2-dimethyl	95-47-6	0.04
116	4-Octen-3-one	14129-48-7	0.00
117	Butane, 1,1'-oxybis-	142-96-1	0.04
118	3-Heptanone	106-35-4	0.14
119	Styrene	100-42-5	0.03
120	Benzene, 1,2-dimethyl	95-47-6	0.03
121	Pentane, 1-methoxy	628-80-8	0.04
122	Cyclohexane,1-ethyl-4-methyl,cis	4926-78-7	0.00
123	Tetramethylcyclohexane		0.01
124	Cyclohexane, 1-ethyl-4-methyl-trans		0.00
125	C8-Alkanone		0.05
126	Mixture		0.01
127	Mixture		0.05
128	Alkanol		0.01
129	Octane, 2,6-dimethyl	2051-30-1	0.11
130	2-Heptanone,4-methyl	6137-06-0	0.03

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
131	Heptane, 3-ethyl, 2-methyl	14676-29-0	0.05
132	Mixture		0.00
133	Octane, 3-methyl	2216-33-3	0.00
134	Cyclooctane, 1,4-dimethyl-, cis-	13151-99-0	0.04
135	3-Heptanone, 6-methyl	624-42-0	0.01
136	2-Heptanone, 6-methyl	928-68-7	0.36
137	Benzene, propyl	103-65-1	0.00
138	Nonane, 4-methyl	17301-94-9	0.07
139	C10-Alkene		0.08
140	Alkanone		0.06
141	C10-Alkene		0.03
142	Octane, 3,5-dimethyl	15869-93-9	0.08
143	Unknown		0.01
144	Alkene		0.03
145	4-Octanone	589-63-9	0.03
146	Cyclopentane,1-methyl-3-(2-methylpropyl	29053-04-1	0.02
147	Phenol	108-95-2	0.05
148	Cyclotetrasiloxane, octamethyl	556-67-2	0.07
149	Cyclopentane, 1,1,3,4-tetramethyl-cis,	53907-60-1	0.01
150	Decane	124-18-5	0.25
151	Mixture		0.02
152	Benzene, 2-propenyl and others		0.01
153	Alkyl-Cyclohexane		0.02
154	C11-Alkane		0.01
155	C6-Cyclopentane		0.02
156	Nonane, 2,6-dimethyl	17302-28-2	0.19
157	Decane, 2-methyl	6975-98-0	0.03
158	1-Hexanol, 2-ethyl	104-76-7	0.02
159	Mixture		0.02
160	Nonane, 3,7-dimethyl	17302-32-8	0.08
161	Mixture		0.04
162	Cyclopentane, 1-hexyl-3-methyl	61142-68-5	0.04
163	Alkanone		0.05

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
164	C12-Alkene		0.13
165	Decane, 4-methyl	2847-72-5	0.05
166	C10-Alkanone		0.19
167	Naphthalene, decahydro-, trans	493-02-7	0.15
168	Ethanone, 1-phenyl	98-86-2	0.01
169	Phenol, 2-methyl and others	95-48-7	0.01
170	alkyl-nitrile		0.02
171	5-Nonanone	502-56-7	0.01
172	Cyclohexane,1,2-diethyl-1-methyl	61141-79-5	0.02
173	C5-Cyclohexane		0.16
174	2-Nonanone	821-55-6	0.13
175	Undecane	1120-21-4	0.61
176	Cyclopentane, 1-methyl-2-(2-propenyl)-trans	50746-53-7	0.01
177	Octane, 6-ethyl-2-methyl	62016-19-7	0.16
178	Undecane, 4-methyl	2980-69-0	0.02
179	Octane,2,5,6-trimethyl	62016-14-2	0.01
180	C11-Alkane		0.01
181	Undecane, 5-methyl	1632-70-8	0.11
182	C12-Alkane		0.06
183	Undecane, 2-methyl	7045-71-8	0.30
184	C12-Alkene		0.01
185	Cyclopropane,1-ethyl-2-heptyl	74663-86-8	0.06
186	Cyclohexane, pentyl	4292-92-6	0.03
187	Cyclohexanone, 5-methyl-2-(1-methylethy	15932-80-6	0.22
188	6-Methylundecane	17302-33-9	0.34
189	Undecane, 4-methyl	2980-69-0	0.15
190	Undecane, 2-methyl	7045-71-8	0.29
191	Undecane, 3-methyl or C12-alkane	1002-43-3	0.15
192	Cyclohexane,1-methyl-4-(1-methylbutyl)-	54411-00-6	0.07
193	Undecane, 2,6-dimethyl	17301-23-4	0.24
194	Dodecane, 4-methyl	6117-97-1	0.06
195	Undecane, 2,10-dimethyl	17301-27-8	0.15
196	Dodecane, 4,6-dimethyl	61141-72-8	0.01

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
197	Tridecane, 2-methyl	1560-96-9	0.11
198	Tridecane, 3-methyl	6418-41-3	0.08
199	Tetradecane	629-59-4	0.23
200	Tridecane, 4,8-dimethyl	55030-62-1	0.02
201	Mixture		0.02
202	C14-Alkene		0.02
203	Tetradecane, 4-ethyl	55045-14-2	0.01
204	C15-Alkane		0.07
205	C15-Alkane		0.05
206	3-Hexadecene, (Z)-	34303-81-6	0.01
207	Pentadecane	629-62-9	0.25
208	Mixture		0.02
209	Tetradecane, 2,6,10-trimethyl	14905-56-7	0.03
210	Dodecane, 2-methyl-6-propyl	55045-08-4	0.04
211	Decane, 3-cyclohexyl-, 3-cyclohexyl-	13151-74-1	0.05
212	Alkanone		0.02
213	Hexadecane	544-76-3	0.11
214	Tridecane, 5-propyl	55045-11-9	0.03
215	Alkane		0.00
216	Alkanone		0.00
217	Heptadecane	629-78-7	0.01
218	Pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.01
219	Tetradecanoic acid	544-63-8	0.01
220	Octadecane	593-45-3	0.00
221	1,1'-Biphenyl, 2,6-dichloro and siloxane		0.00
222	Benzenesulfonamide, N-butyl	3622-84-2	0.04
223	Alkane		0.00
224	9-Hexadecenoic acid	2091-29-4	0.00
225	Hexadecanoic acid	57-10-3	0.01
226	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.01
227	Alkane		0.00

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero.

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