DISTRIBUTION SHEET

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Distribution	J. W. Osborne	Date May 31, 1995
Project Title/Work Order		EDT No.
Tank 241-BY-106 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-420)		ECN No. 623543

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 623543

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.
	WHC-SD-WM-ER-420, Rev 0	N/A	N/A

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)

See attached distribution sheet

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DATE MAY 31 1995

STA 4

A-7900-013-2 (11/94) GEF095

ENGINEERING CHANGE NOTICE

1. ECN (use no. from pg. 1) 623543

15. Design Verification Required
[] Yes
[X] No

16. Cost Impact

	ENGINEERING		CONSTRUCTION	
Additional	[]	$	[]	$
Savings	[]	$	[]	$

17. Schedule Impact (days)

Improvement	[]
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18. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 12. Enter the affected document number in Block 19.

SDD/DD	[]	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 J. W. Osborne	5-31-95	PE	
Cog. Mgr. T. J. Kelley 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-420 REV 1
Document Title:	Tank 241-BY-106 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 25

2. Title	3. Number	4. Rev No.
Tank 241-BY-106 Vapor Sampling and Analysis Tank Characterization Report	WHC-SD-WM-ER-420	1

5. Key Words	6. Author
241-BY-106, Headspace vapor samples, organic analytes, VSS, SUMMA™, inorganic gases and vapors	Name: J. L. Huckaby Signature J L Huckaby Organization/Charge Code 75600/N4AB1

7. Abstract

Tank 241-BY-106 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-106 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).

DISCLAIMER

8. RELEASE STAMP

RECORD OF REVISION	(1) Document Number WHC-SD-WM-ER-420	Page 1

(2) Title

Tank 241-BY-106 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
1 RS	(7) Made editorial changes and added ECN-623543 information in organic vapor chapter.	J.W.Osborne	T.J.Kelley 5-31-95
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Tank 241-BY-106 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank BY-106 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-106 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 gas and vapor samples were collected from tank BY-106 using the vapor sampling system (VSS) on July 8, 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 BY-106 headspace was withdrawn via a heated sampling probe mounted in riser 10B, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 65 °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 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 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, and SUMMA™ canisters were analyzed for inorganic analytes by

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

OGIST. Reports by PNL (Lucke et al. 1994) and SNL/OGIST (Rasmussen 1994a and 1994b) 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 1 % for nitrous oxide results, to 28 % for nitric oxide results. The larger relative standard deviation of the nitric oxide results is due to the fact that it is very near the analytical method's limit of quantitation. 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, 74 ppmv, is about 3 times higher than the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995). 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 45.5 ppmv of hydrogen in tank BY-106, however, represents only about 0.1 % 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-106, 70.6 ppmv, is about 3 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, 47.6 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. 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. 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 1994c, 1994d).

Carbon monoxide in the tank BY-106 headspace, at about 0.45 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 product of organic waste in the

tank. Tanks known to have significantly higher organic vapor concentrations have also been observed to have higher carbon monoxide concentrations (e.g., carbon monoxide concentration in C-103 was 26.7 ppmv, Huckaby and Story 1994). With a NIOSH 8-hr REL of 35 ppmv (NIOSH 1995), the 0.45 ppmv in tank BY-106 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-106 headspace were determined to be 0.13 ppmv and 0.05 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH interstitial liquid in tank BY-106. 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-106 was determined to be about 14.7 mg/L, at the tank headspace temperature of 27 °C and pressure of 984 mbar (740 torr), (WHC 1995). This corresponds to water vapor partial pressure of 20.4 mbar (15.3 torr), to a dew point of 17.8 °C, and to a relative humidity of 57 %.

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 34 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-106 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. (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 1994a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-106. 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, and their average concentrations from the analysis of 4 TSTs, are given in Table X-3. The TST target analytes for tank BY-106 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 7 of the 40 TO-14 analytes were observed to be above the 0.002 ppmv quantitation limit of the analyses (Lucke 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 are in excellent agreement for dichloromethane and toluene, but differ by more than a factor of 3 for benzene. Though the benzene values differ by more than the allowed ±30 % analytical accuracy, this difference is reasonable given that fundamentally different sampling devices and analytical methods were used. What is important in this case is that both ORNL and PNL results, 0.0073 ppmv and 0.0022 ppmv respectively, clearly indicate that benzene is well below its NIOSH STEL of 1 ppmv.

The 3 most abundant organic compounds in the tank BY-106 headspace are methane, acetone, and 1-butanol. At 3.6 ppmv, the methane concentration is about 2 times higher than its normal ambient air concentration. Methane is probably formed during the chemical and radiolytic degradation of organic wastes in the tank. Methane is not a constituent of toxicological concern, and its LFL in air is about 5 % by volume. This places the 3.6 ppmv of methane in tank BY-106 at about 0.007 % of its LFL. Acetone, at 0.37 ppmv, and 1-butanol, at 0.34 ppmv, similarly present virtually no flammable or toxicological risks.

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 Lucke 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 chromatographic peak doublets and even triplets (e.g., Cmpd # 2, 3, and 4 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 9,900 $\mu g/m^3$, with a standard deviation of 350 $\mu g/m^3$. Though data on other tanks is very limited, this value is neither high nor low compared to most other waste tanks sampled to date.

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. The specific presence of the decahydronaphthalenes and cyclohexanes, which were not observed in tank C-103 samples, is an indication of their different waste histories.

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-106 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	5.0	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	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-106 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	74	2	3
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	47.6	1.4	3
Carbon Monoxide, CO	630-08-0	SUMMA™	3	0.45	.03	7
Hydrogen, H_2	1333-74-0	SUMMA™,[3]	3	45.5	2.5	5
Nitric Oxide, NO	10102-43-9	Sorbent Trap	10	0.13	0.04	28
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap™,[4]	5	0.05	0.006	13
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	70.6	0.6	1
Water Vapor, H_2O	7732-18-5	Sorbent Trap	10	20,700 (14.7 mg/L)	1,200 (0.8 mg/L)	6

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. Hydrogen analysis of 7/8/94 samples problematic, average given is for 3 SUMMA™ canister samples collected 5/4/94 (Rasmussen 1994b).

4. Only 5 of the 10 samples were statistically above blank NO_2 levels.

Table X-3
Tank BY-106 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]	3.6	<0.1	4
Dichlorodifluoromethane	75-71-8	SUMMA™	0.011	0.002	18
Chloromethane (Methyl chloride)	74-87-3	SUMMA™	0.0028	0.0006	20
Trichlorofluoromethane	75-69-4	SUMMA™	0.19	0.02	9
Dichloromethane (Methylene chloride)	75-09-2	TST[4]	0.00047	0.00017	36
		SUMMA™	<0.002	--	--
Ethanenitrile (Acetonitrile)	75-05-8	TST	0.12	0.02	16
Propanone (Acetone)	67-64-1	TST	0.37	0.08	23
Propanenitrile	107-12-0	TST	0.0043	0.0002	5
Butanal	123-72-8	TST	0.061	0.013	21
n-Hexane	110-54-3	TST	0.085	0.011	13
Benzene	71-43-2	TST	0.0073	0.0008	11
		SUMMA™	0.0022	0.0004	19
1-Butanol	71-36-3	TST	0.34	0.03	8
Butanenitrile	109-74-0	TST	0.0015	0.00009	6
2-Pentanone	107-87-9	TST	0.011	0.0009	9
n-Heptane	142-82-5	TST	0.031	0.002	6
Toluene	108-88-3	TST	0.0083	0.0011	13
		SUMMA™	0.0071	0.0003	5
Tetrachloroethene	127-18-4	SUMMA™	0.003	0.001	34
Ethylbenzene	100-41-4	SUMMA™	0.0013[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™	0.0031	0.0004	13
Pentanenitrile	110-59-8	TST	0.0010	0.0001	11
2-Hexanone	591-78-6	TST	0.0042	0.0005	13
n-Octane	111-65-9	TST	0.012	0.001	11
Hexanenitrile	628-73-9	TST	0.00072	0.00011	15
2-Heptanone	110-43-0	TST	0.0032	0.0007	23
n-Nonane	111-84-2	TST	0.0046	0.0006	14
Heptanenitrile	629-08-3	TST	0.00034	0.00003	9
2-Octanone	111-13-7	TST	0.00094	0.00029	31
Octanenitrile	124-12-9	TST	0.00018	0.00002	9
Nonanenitrile	2243-27-8	TST	0.00019	0.00003	15
n-Dodecane	112-40-3	TST	0.0065	0.0014	22
n-Tridecane	629-50-5	TST	0.0069	0.0019	28
Tributyl phosphate (TBP)	126-73-8	TST	0.000044	0.000009	20
Dibutyl butylphosphonate (DBBP)	75-46-4	TST	0.0000064	0.0000030	47

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. All SUMMA canister results are based on analyses of 3 samples. SUMMA™ analysis of methane were performed by OGIST, other SUMMA™ analyses in this table were performed by PNL.

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

5. Result of single sample, other samples <0.002 ppmv.

Table X-4
Tank BY-106 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
1	Propene	115-07-1	1.04	0.18
2	Propane	74-98-6	0.68	0.14
3	Propyne		0.06	0.01
4	Cyclopropane	75-19-4	0.17	0.04
5	2-Methylpropane	75-28-5	0.56	0.24
6	2-Methylpropene	115-11-7	0.73	0.27
7	n-Butane	106-97-8	0.86	0.35
8	2-Butene	107-01-7	0.16	0.07
9	Ethanol[2]	64-17-5	0.11	--
10	C4 Alkene		0.09	0.04
11	Acetone	67-64-1	0.88	0.46
12	C5 Alkane		0.40	0.24
13	1-Pentene	109-67-1	0.25	0.11
14	n-Pentane	109-66-0	0.75	0.44
15	C5 Alkene[1]		0.06	--
16	C6 Alkene[1]		0.08	--
17	1-Pentanol[1]	71-41-0	0.07	--
18	2-Methylpentane	107-83-5	0.71	0.06
19	Butanal	123-72-8	0.17	0.04
20	2-Butanone (MEK)	78-93-3	0.17	0.03
21	3-Methylpentane	96-14-0	0.14	0.01
22	1-Hexene	592-41-6	0.15	0.02
23	n-Hexane	110-54-3	0.54	0.08
24	Tetrahydrofuran	109-99-9	0.17	0.02
25	2-Methyl-1-pentene	763-29-1	0.07	0.01
26	1-Butanol	71-36-3	0.99	0.13
27	2-Pentanone	107-87-9	0.13	0.02

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
28	C7 Alkane		0.24	0.05
29	1-Heptene	592-76-7	0.06	0.01
30	n-Heptane	142-82-5	0.33	0.04
31	C7 Alkene		0.06	0.01
32	C8 Alkane		0.12	0.02
33	Hexanal[1]	66-25-1	0.07	--
34	n-Octane	111-65-9	0.11	0.02
35	2-Butoxyethanol[1]	111-76-2	0.06	--
36	C10 Alkane		0.06	0.01
37	C10 Alkane[1]		0.05	--
38	Phenol[1]	108-95-2	0.05	--
39	C11 Alkane[1]		0.05	--
40	n-Undecane	1120-21-4	0.06	0.00
41	n-Dodecane	112-70-3	0.09	0.01
42	C12 Alkane		0.07	0.01
43	Benzothiazole[1] (impurity)	95-16-9	0.06	--
44	C7 Cyclohexane[1]		0.06	--
45	C13 Alkane		0.06	0.01
46	n-Tridecane	629-50-5	0.09	0.01
47	C13 Alkane		0.06	0.01
48	C13 Alkane		0.06	0.01

1. CAS = Chemical Abstract Service.

2. Detected in only 1 sample.

Table X-5
Tank BY-106 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
1	2-Butene, (Z)-	107-01-7	0.527
2	1-Propene, 2-methyl-	115-11-7	0.040
3	1-Propene, 2-methyl-	115-11-7	0.125
4	1Propene, 2-methyl-	115-11-7	0.035
5	1-Butene, 3-methyl-	563-45-1	0.053
6	Methyl ether	115-10-6	0.133
7	Butane, 2-methyl-	78-78-4	0.298
8	Methane, trichlorofluoro-	75-69-4	0.265
9	1-Pentene	109-67-1	0.297
10	1-Butyne and others	107-00-6	0.004
11	Propane, 2-methyl-	75-28-5	1.685
12	Furan	110-00-9	0.028
13	1,3-Pentadiene, (E)- and C5-Alkene	2004-70-8	0.017
14	2-Propanol	67-63-0	0.276
15	2-Pentene, (Z)-	627-20-3	0.016
16	Cyclopentane	287-92-3	0.076
17	Cyclopropane, 1,1-dimethyl-	1630-94-0	0.026
18	1-Pentyne and C4-alkene	627-19-0	0.018
19	1,3-Pentadiene, (Z)-	504-60-9	0.027
20	Butane, 2,2-dimethyl-	75-83-2	0.005
21	2-Propenenitrile and others	107-13-1	0.007
22	1-Pentene, 4-methyl-	691-37-2	0.109
23	Cyclopentane	287-92-3	0.048
24	Pentane, 2-methyl-	107-83-5	0.699
25	C3-cyclopropane		0.045
26	2,3-Dihydrofuran		0.035
27	Cyclopropane, propyl-	2415-72-7	0.004
28	1-Butene	106-98-9	0.005
29	Pentane, 3-methyl-	96-14-0	0.152
30	Propanenitrile	107-12-0	0.006
31	1-Pentene, 2-methyl-	763-29-1	0.068

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
32	C6-alkene		0.169
33	3-Buten-2-one	78-94-4	0.036
34	2-Butanone	78-93-3	0.212
35	2-Hexene, (Z)-	7688-21-3	0.023
36	2-Pentene, 4-methyl-, (E)-	674-76-0	0.029
37	Alkanol		0.032
38	Cyclopropane, propyl-	2415-72-7	0.116
39	C6-alkene		0.025
40	Cyclopentane, methyl-	96-37-7	0.096
41	Alkenol		0.158
42	Furan, tetrahydro-	109-99-9	0.302
43	1,3-Butadiene, 2,3-dimethyl-	513-81-5	0.048
44	1,4-Hexadiene	592-45-0	0.033
45	1H-Pyrrole and others	109-97-7	0.008
46	Mixture		0.007
47	1-Hexene, 5-methyl-	3524-73-0	0.028
48	2-Butenal	4170-30-3	0.015
49	Furan, 2,5-dihydro-	1708-29-8	0.029
50	3-Butenenitrile	109-75-1	0.016
51	Hexane, 2-methyl-	591-76-4	0.044
52	1-Hexene, 3,4-dimethyl-	16745-94-1	0.003
53	Pentane, 2,3-dimethyl-	565-59-3	0.001
54	Furan, 2-propyl-	4229-91-8	0.340
55	Cyclopentane, 1,3-dimethyl-, cis-	2532-58-3	0.002
56	C3-Cyclopentane		0.002
57	C6-alkenone		0.008
58	Cyclopentane, 1,2-dimethyl-	2452-99-5	0.010
59	C2-cyclopentane		0.066
60	2-Pentanol	6032-29-7	0.009
61	2-Heptene, (E)-	14686-13-6	0.005
62	2-Pentanone, 4-methyl-	108-10-1	0.010
63	2-Heptene	592778	0.001
64	Cyclohexane, methyl-	108-87-2	0.041

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
65	1-Hexene, 2-methyl-	6094-02-6	0.001
66	Hexane, 2,4-dimethyl-	589-43-5	0.001
67	C7-alkene		0.010
68	2-Pentanol, 2-methyl-	590-36-3	0.013
69	C6-Alkenone		0.001
70	C8-Alkene		0.002
71	2-Pentanone, 4-methyl-	108-10-1	0.010
72	Alkane		0.006
73	Mixture		0.001
74	Mixture		0.005
75	Cyclopropane, 1-heptyl-2methyl-	74663-91-5	0.015
76	C8-Alkene		0.001
77	Pentane, 3-ethyl-2-methyl-	609-26-7	0.024
78	Heptane, 3-methyl-	589-81-1	0.055
79	1-Octen-3-one	4312-99-6	0.017
80	Cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.007
81	C2-cyclohexane		0.001
82	1,4-Hexadiene, 4-methyl- and others	1116-90-1	0.001
83	3-Hexanone	589-38-8	0.016
84	1-Hexene, 4,5-dimethyl-	16106-59-5	0.001
85	Hexanal	66-25-1	0.010
86	Formamide, N-(2-methylpropyl)-	6281-96-5	0.007
87	Alkanol		0.003
88	1-Pentanol, 5-methoxy-	4799-62-6	0.003
89	Cyclopentane, 1,1,3-trimethyl-	4516-69-2	0.005
90	Hexanal	66-25-1	0.003
91	Ethene, tetrachloro-	127-18-4	0.023
92	Acetic acid, butyl ester	123-86-4	0.007
93	Hexamethylcyclotrisiloxane	541-05-9	0.006
94	Pyridine, 4-methyl-	108-89-4	0.007
95	Nitric acid, butyl ester	928-45-0	0.000
96	Heptane, 2,6-dimethyl-	1072-05-5	0.022
97	2-Pentanol, 2,3-dimethyl-	4911-70-0	0.005

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
98	4-Heptenal, (Z)-	6728-31-0	0.002
99	Cyclohexane, ethyl-	1678-91-7	0.011
100	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.019
101	Hexane, 3-methoxy-	54658-01-4	0.009
102	7-Octen-2-one	3664-60-6	0.007
103	Cyclobutanone, 2,3,3-trimethyl-	28290-01-9	0.011
104	Cyclohexane, 1,3,5-trimethyl-	1839-63-0	0.006
105	Heptane, 2,3-dimethyl-	3074-71-3	0.012
106	Octane, 2-methyl-	3221-61-2	0.020
107	Nirto-Compound		0.001
108	Octane, 3-methyl-	2216-33-3	0.024
109	Benzene, 1,3-dimethyl-	108-38-3	0.020
110	4-Octen-3-one	14129-48-7	0.001
111	Cyclohexane, 1,2,3-trimethyl-	1678-97-3	0.001
112	Alkane		0.015
113	C3-cyclohexane and others		0.004
114	Acetamide, N,N-dimethyl- and others	127-19-5	0.001
115	3-Heptanone	106-35-4	0.028
116	Styrene	100-42-5	0.005
117	Benzene, 1,4-dimethyl-	106-42-3	0.008
118	Heptanal	111-71-7	0.007
119	Cyclohexane, 1,1,3,5-tetramethyl-, trans-	50876-31-8	0.001
120	C3-Cyclohexane		0.001
121	Cyclohexane, 1-ethyl-4-methyl-, cis	4926-78-7	0.004
122	C7-alkanone		0.005
123	Mixture		0.002
124	Cyclopropene, 1-butyle-2-ethyl-	50915-91-8	0.016
125	Cyclohexanol, 3-methyl- and others	591-23-1	0.001
126	2-Heptanol, 2-methyl-	625-25-2	0.003
127	Octane, 2,6-dimethyl-	2051-30-1	0.022
128	Cyclohexane, (1-methylethyl)-	696-29-7	0.002
129	Pyridine, 3,5-dimethyl- and others	591-22-0	0.004
130	Furan and others	110-00-9	0.001

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
131	Heptane, 3-ethyl-2-methyl-	14676-29-0	0.006
132	Mixture		0.003
133	2-Heptanone, 6-methyl-	928-68-7	0.031
134	Benzene, propyl-	103-65-1	0.003
135	Nonane, 4-methyl-	17301-94-9	0.012
136	1,1,2,3-tetramethylcyclohexane A		0.024
137	Alkenol		0.034
138	Alkene		0.010
139	C3-cyclohexene		0.003
140	3-Pentene-2-ol and others	1569-50-2	0.002
141	4-Octanone and others	589-63-9	0.002
142	Cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	0.006
143	C3-Cyclohexene		0.001
144	Cyclohexane, 1-methyl-4-(-methylethyl)-, cis-	6069-98-3	0.006
145	Phenol	108-95-2	0.010
146	Cyclotetrasiloxane, octamethyl-	556-67-2	0.024
147	Butanoic acid, butyl ester	109-21-7	0.005
148	Decane	124-18-5	0.049
149	4-Nonene, 5-methyl-	15918-07-7	0.001
150	(Z)-2,3,4,5-tetramethyl-3-hexene		0.005
151	C5-cyclopentane		0.002
152	C4-Cyclohexane		0.001
153	Cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	0.004
154	Heptane, 2,3,6-trimethyl-	4032-93-3	0.004
155	3-Hexane, 2,2,5,5-tetramethyl-, (A)- and others		0.006
156	Nonane, 2,6-dimethyl-	17302-28-2	0.034
157	Cyclohexanol, 4-(1,1,3,3-tetramethylbutyl)-	4631-98-5	0.004
158	1-Hexanol, 2-ethyl	104-76-7	0.001
159	Undecane	1120-21-4	0.005
160	Cyclohexane, (1-methylpropyl)-	7058-01-7	0.014
161	Cyclopentane, 1-hexyl-3-methyl-	61142-68-5	0.001
162	1,1,2,3-Tetramethylcyclohexane A		0.001

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
163	C5-cyclohexane		0.004
164	C4-cyclohexane		0.008
165	1-Undecene	821-95-4	0.001
166	Mixture		0.001
167	Cyclohexanone, 2,6-diethyl-	16519-68-9	0.001
168	1,1-dimethyl-2-propylcyclohexane		0.017
169	Decane, 4-methyl-	2847-72-5	0.006
170	Decane, 2,6,7-trimethyl-	62108-25-2	0.016
171	Naphthalene, decahydro-, trans-	493-02-7	0.024
172	Mixture		0.001
173	Ethanone, 1-phenyl-	98-86-2	0.010
174	1-Naphthalenol, decahydro-4a-methyl-8-methylene-2-(1-met) and others	30951-17-8	0.007
175	C5-cyclohexane		0.007
176	Cyclohexane, 1,2-diethyl-1-methyl-Zinc, bis[2-(1,1-dimethylethyl)-3,3-dimethylcyclopro	61141-79-5	0.005
177	C5-cyclohexane		0.016
178	2-Nonanone	821-55-6	0.004
179	C6-cyclohexane		0.005
180	Undecane	1120-21-4	0.071
181	5-Undecene	4941-53-1	0.005
182	C11-alkene		0.006
183	Cyclopropane, octyl-	1472-09-9	0.004
184	Undecane, 5-methyl-	1632-70-8	0.012
185	Cyclohexene, 1-pentyl-	15232-85-6	0.006
186	Naphthalene, decahydro-2-methyl-	2958-76-1	0.030
187	C6-Alkenyl-cyclopentane		0.001
188	5-Dodecene, (Z)-	7206-28-2	0.006
189	Benzoic acid, 2-[(trimethylsilyl)oxyl-, trimethylsilyl ester	3789-85-3	0.004
190	Cyclohexane, pentyl-	4292-92-6	0.014
191	Naphthalene, decahydro-2-methyl-	2958-76-1	0.025
192	Decane, 2,4-dimethyl-	2801-84-5	0.003

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
193	6-Methylundecane	17302-33-9	0.023
194	Undecane, 4-methyl-	2980-69-0	0.012
195	Undecane, 2-methyl-	7045-71-8	0.019
196	C6-cyclohexane		0.006
197	Undecane, 3-,methyl-	1002-43-3	0.009
198	2-Cyclohexen-1-one, 4-ethyl-3,4-dimethyl-	17622-46-7	0.003
199	2-Propyl-1,1,3-trimethylcyclohexane		0.005
200	Naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.007
201	Decane, 2,3,6-drimethyl-	62238-12-4	0.007
202	Mixture		0.001
203	Cyclohexane, 1,-methyl-3-pentyl-	54411-02-8	0.002
204	Cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.006
205	Naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.001
206	Cyclohexane, 1-ethyl-2-methyl-, cis-	4923-77-7	0.016
207	Undecane, 2,6-dimethyl-	17301-23-4	0.027
208	C2-Decahydronaphthalene		0.005
209	Undecane, 4,8-dimethyl-	17301-33-6	0.006
210	C2-Decahydronaphthalene		0.003
211	Naphthalene, decahydro-1,5-dimethyl-	66552-62-3	0.010
212	4-Nonene, 5-butyl-	7367-38-6	0.019
213	(E,E)(3S,8S),3,8-dimethyldeca-4,6-diene		0.015
214	C7-Cyclohexane		0.002
215	Naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.001
216	C7-Cyclohexane		0.009
217	Undecane, 2,10-dimethyl-	17301-27-8	0.019
218	Tridecane, 7-methyl-	26730-14-3	0.049
219	Cyclohexane, 1,2-diethyl-3-methyl-	61141-80-8	0.007
220	2(3H)-Benzofuranone, 3a,4,5,6-tetrahydro-3a,6,6-trimethyl-	16778-26-0	0.010
221	6-Tridecane, 7-methyl-	24949-42-6	0.022
222	Phenol, 4-(1,1-dimethylethyl)- and others	98-54-4	0.004
223	Cyclohexane, (2-ethyl-1-methyl-1-butenyl)-	74810-42-7	0.002
224	Undecane, 6-ethyl-	17312-60-6	0.001

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
225	Dodecane, 2,5-dimethyl-	56292-65-0	0.010
226	C8-Cyclohexane		0.004
227	C8-Cyclohexane		0.006
228	7-Tetradecene	10374-74-0	0.004
229	2-Octylfuran		0.006
230	Cyclohexane, octyl-	1795-15-9	0.012
231	Tridecane, 4-methyl-	26730-12-1	0.005
232	Tridecane, 2-methyl-	1560-969	0.006
233	C1-acridine and others		0.021
234	Dodecane, 2,6,10-trimethyl-	3891-98-3	0.061
235	Tetradecane	629-59-4	0.045
236	Tridecane, 4,8-dimethyl-	55030-62-1	0.012
237	1,1,2,3-tetramethylcyclohexane A		0.019
238	Cyclopentane, (1-methylbutyl)-	4737-43-3	0.007
239	Cyclohexane, 1,1,3,5-tetramethyl-, cis-	50876-32-9	0.001
240	1-Pentadecene	13360-61-7	0.001
241	Alkane		0.001
242	C16-Alkane		0.006
243	Dodecane, 2-methyl-8-propyl-	55045-07-3	0.057
245	Pentadecane, 2-methyl-	1560-93-6	0.003
246	Alkane		0.004
247	3-tert-butyl-4-methoxphenol	88-32-4	0.000
248	Phenol, (1,1-dimethylethyl)-4-methoxy-	25013-16-5	0.001
249	7-Hexadecene, (Z)-	35507-09-6	0.010
250	Pentadecane	629-62-9	0.043
251	3,4-Undecadiene-2,10-dione, 6,6-dimethyl-	52588-78-0	0.000
252	C9-Cyclohexane		0.000
253	Tridecane, 2-methyl-	1560-96-9	0.005
254	Alkane		0.004
255	Alkane		0.005
256	Alkane		0.000
257	Hexadecane, 3-methyl-	6418-43-5	0.001
258	5-Undecanone, 2-methyl-	50639-02-6	0.001

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
259	Hexadecane	544-76-3	0.015
260	1,2-Benzenedicarboxylic acid, diethyl ester	84-66-2	0.038
261	Pentadecane, 2,6,10-dimethyl-		0.006
262	1-Hexadecanol	36653-82-4	0.003
263	Heptadecane	629-78-7	0.003
264	Pentadecane, 2,6,10,14-tetramethyl-	1921-70-6	0.004
265	Alkane		0.004
266	1,1'-Biphenyl, 2,2'-diethyl-	13049-35-9	0.000
267	Tetradecanoic acid	544-63-8	0.008
268	Benzenesulfonamide, N-butyl-	3622-84-2	0.034
269	Pentadecanoic acid	1002-84-2	0.002
270	1-Hexadecanol	36653-82-4	0.003
271	Alkene and others		0.004
272	Hexadecanoic acid	57-10-3	0.013
273	Pathalate		0.001
274	Hexadecanoic acid	57-10-3	0.003

1. CAS = Chemical Abstract Service.

2. Average includes samples with zero concentration.

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