DISTRIBUTION SHEET

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Distribution	J. W. Osborne	Date May 31, 1995
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Tank 241-BY-105 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-419)		ECN No. 623542

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

ENGINEERING CHANGE NOTICE

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1. ECN No 623542

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
	8. Document Numbers Changed by this ECN (includes sheet no. and rev.) WHC-SD-WM-ER-419, Rev 0	9. Related ECN No(s).	10. Related PO No. 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)

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

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1. ECN (use no. from pg. 1): 623542

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	[]
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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-419 REV 1
Document Title:	Tank 241-BY-105 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 26

2. Title	3. Number	4. Rev No.
Tank 241-BY-105 Vapor Sampling and Analysis Tank Characterization Report	WHC-SD-WM-ER-419	1

5. Key Words	6. Author
241-BY-105, 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-105 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-105 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-419	Page 1

(2) Title

Tank 241-BY-105 Vapor Sampling and Analysis Tank Characterization Report

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release	
	EDT-607553	(5) Cog. Engr.	(6) Cog. Mgr. Date
RS 1	(7) Made editorial changes and added information in organic vapor chapter.	J.W.Osborne	T.M.Kelley 5-31-95
	ECN-623542		

Tank 241-BY-105 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank BY-105 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-105 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-105 using the vapor sampling system (VSS) on July 7, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by the sample and analysis plan (Appendix A, WHC 1995). The tank headspace temperature was determined to be 26 °C. Air from the tank BY-105 headspace was withdrawn via a heated sampling probe mounted in riser 10A, 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 (Pool et al. 1995) and SNL/OGIST (Rasmussen 1994a, 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 0.6 % for nitrous oxide results, to 27 % 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, 43 ppmv, is 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 have been observed to exceed 1000 ppmv (McVeety et al. 1995). The 43 ppmv ammonia concentration in tank BY-105 is lower than that in most other tanks sampled to date.

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 47.9 ppmv of hydrogen in tank BY-105, 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-105, 49.5 ppmv, is about 2 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, 94 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-105 headspace, at about 0.38 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, the 0.45 ppmv in tank BY-105 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-105 headspace were determined to be 0.10 ppmv and ≤ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH interstitial liquid in tank BY-105. 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-105 was determined to be about 14.9 mg/L at the measured headspace temperature of 26 °C and pressure of 991 mbar (745 torr), (WHC 1995). This corresponds to water vapor partial pressure of 20.6 mbar (15.5 torr), to a dew point of 18.0 °C, and to a relative humidity of about 61 %.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Analysis of the silica gel indicated the total activity of the headspace to be below 50 pCi/L (WHC 1995).

X.3 ORGANIC VAPORS

Organic vapors in the tank BY-105 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 Pool 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 BY-105. 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-105 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, Pool et al. 1995). Only 4 of the 40 TO-14 analytes were observed to be above the 0.002 ppmv quantitation limit of the analyses (Pool et al. 1995 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 differ by more than the allowed ±30 % analytical accuracy, however, 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 (0.0052 and <0.002 ppmv for dichloromethane, 0.0069 and <0.002 ppmv for benzene, and 0.0086 and 0.0024 ppmv for toluene, respectively) clearly indicate that dichloromethane, benzene, and toluene are well below their Occupational Safety and Health Administration (OSHA) permissible exposure levels (PELs) for time weighted averages (TWAs) of 500, 1, and 200 ppmv, respectively (NIOSH 1995).

The 3 most abundant organic compounds in the tank BY-105 headspace are methane, 1-butanol, and acetone. At 3.8 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 3.8 ppmv of methane in tank BY-105 at about 0.008 % of its LFL. 1-Butanol, at 0.70 ppmv, and acetone, at 0.25 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 lists the compounds tentatively identified by PNL, 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 mass spectral (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 Pool et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-4 and X-5 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 3, 4, and 5 in Table X-5). In these instances, the estimated concentration of a compound split into multiple 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 1994a). The sample mean was 12,650 $\mu g/m^3$, with a standard deviation of 380 $\mu g/m^3$. 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-105 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	4.0	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-105 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	43	1	2
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	94	2	2
Carbon Monoxide, CO	630-08-0	SUMMA™	3	0.38	0.04	11
Hydrogen, H_2	1333-74-0	SUMMA™,[3]	3	47.9	1.1	2
Nitric Oxide, NO	10102-43-9	Sorbent Trap	10	0.10	0.03	27
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	10	≤ 0.02	--	--
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	49.5	0.3	0.6
Water Vapor, H_2O	7732-18-5	Sorbent Trap	10	20,800 (14.9 mg/L)	500 (0.3 mg/L)	2

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. Hydrogen analyses of 7/794 samples was problematic, average given is for 3 SUMMA™ canisters samples collected 5/9/94 (Rasmussen 1994b).

Table X-3
Tank BY-105 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]	3.8	<0.1	<3
Dichlorodifluoromethane	75-71-8	SUMMA™	0.002[4]	--	--
Trichlorofluoromethane	75-69-4	SUMMA™	0.044	0.006	13
Dichloromethane (methylene chloride)	75-09-2	TST[5]	0.0052	0.0010	19
		SUMMA™	<0.002	--	--
Ethanenitrile (acetonitrile)	75-05-8	TST	0.081	0.011	14
Propanone (acetone)	67-64-1	TST	0.25	0.02	7
Propanenitrile	107-12-0	TST	0.0017	0.0004	22
Butanal	123-72-8	TST	0.047	0.008	16
n-Hexane	110-54-3	TST	0.086	0.009	10
Benzene	71-43-2	TST	0.0069	0.0007	11
		SUMMA™	<0.002	--	--
1-Butanol	71-36-3	TST	0.70	0.11	16
Butanenitrile	109-74-0	TST	0.0010	0.0001	12
2-Pentanone	107-87-9	TST	0.012	0.002	14
n-Heptane	142-82-5	TST	0.039	0.003	8
Toluene	108-88-3	TST	0.0086	0.0011	13
		SUMMA™	0.0024	0.0002	9
1,3-Dimethylbenzene (m-xylene) + 1,4-Dimethylbenzene (p-xylene)	108-38-3 106-42-3	SUMMA™	0.0023	0.0001	3
Pentanenitrile	110-59-8	TST	0.00079	0.00008	10

Compound	CAS[1] Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
2-Hexanone	591-78-6	TST	0.0054	0.0007	12
n-Octane	111-65-9	TST	0.015	0.001	8
Hexanenitrile	628-73-9	TST	0.00085	0.00016	19
2-Heptanone	110-43-0	TST	0.0044	0.0006	13
n-Nonane	111-84-2	TST	0.0060	0.0006	10
Heptanenitrile	629-08-3	TST	0.00049	0.00004	7
2-Octanone	111-13-7	TST	0.0010	0.0002	19
Octanenitrile	124-12-9	TST	0.00026	0.00002	7
Nonanenitrile	2243-27-8	TST	0.00031	0.00004	14
n-Dodecane	112-40-3	TST	0.0081	0.0008	10
n-Tridecane	629-50-5	TST	0.010	0.002	15
Tributyl phosphate (TBP)	126-73-8	TST	0.00017	0.00013	76
Dibutyl butylphosphonate (DBBP)	75-46-4	TST	0.000025	0.000013	52

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

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

4. Average of 2 samples, other sample result <0.002 ppmv.

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

Table X-4
Tank BY-105 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	0.96	0.19
2	Propane	74-98-6	0.28	0.04
3	Cyclopropane[2]	75-19-4	0.07	0.01
4	2-Methylpropane	75-28-5	0.16	0.04
5	2-Methylpropene	115-11-7	0.34	0.07
6	n-Butane	106-97-8	0.25	0.05
7	C4 Alkene		0.06	0.01
8	2-Methyl-1-butene[3]	563-46-2	0.05	--
9	Propanone (acetone)	67-64-1	0.16	0.04
10	2-Methylbutane	78-78-4	0.09	0.02
11	2-Pentene	109-68-2	0.12	0.02
12	C5 Alkane		0.19	0.04
13	2-Methylpentane	107-83-5	0.47	0.07
14	2-Butanone	78-93-3	0.07	0.01
15	3-Methylpentane	96-14-0	0.09	0.01
16	1-Hexene	107-01-7	0.14	0.02
17	n-Hexane (coeluent with an internal standard)	110-54-3	0.34	0.06
18	Unknown		0.12	0.02
19	C6 Alkene[1]		0.06	0.01
20	1-Butanol	71-36-3	0.53	0.08
21	C7 Alkane		0.07	0.01
22	C7 Alkane		0.14	0.01
23	1-Heptene	592-76-7	0.06	0.01
24	n-Heptane	142-82-5	0.22	0.03
25	2-Methylheptane	592-27-8	0.08	0.01
26	2,4-Dimethylhexane	589-43-5	0.08	0.01

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
27	Siloxane[2]		0.14	--
28	2-Butoxyethanol[1]	111-76-2	0.06	0.01
29	Siloxane[2]		0.07	--
30	n-Dodecane	112-70-3	0.09	0.01
31	C13 Alkane		0.07	0.01
32	C13 Alkane		0.09	0.02
33	n-Tridecane	629-50-5	0.14	0.03
34	C14 Alkane		0.12	0.02
35	n-Tetradecane	629-59-4	0.13	0.03
36	Unknown		0.08	0.02
37	Unknown[2]		0.05	--
Sum of tentatively identified compounds:			5.96	

1. CAS = Chemical Abstract Service.

2. Detected in only 2 samples.

3. Detected in only 1 sample.

Table X-5
Tank BY-105 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
1	1-Butene or C4-alkene	106-98-9	0.57
2	Butane	106-97-8	0.47
3	1-Propene,2-methyl or C4-alkene	115-11-7	0.08
4	1-Propene,2-methyl- or C4 alkene	115-11-7	0.07
5	1-Propene,2-methyl or C4-alkene	115-11-7	0.07
6	1-Butene,3-methyl	563-45-1	0.07
7	Methane, oxybis (methyl ether)	115-10-6	0.03
8	C5-alkane		0.21
9	Methane, trichlorofluoro	75-69-4	0.14
10	2-Pentene, (Z)	627-20-3	0.01
11	1-Pentene	109-67-1	0.38
12	Furan	110-00-9	0.04
13	C5-alkene and C5-alkyne		0.20
14	2-Pentene, (Z)	627-20-3	0.04
15	Cyclopropane, ethyl	1191-96-4	0.06
16	Cyclopropane, 1,1-dimethyl	1630-94-0	0.03
17	1-Pentyne and C5-alkene	627-19-0	0.01
18	1,2-Pentadiene	591-95-7	0.03
19	1,3-Butadiene, 2-methyl	78-79-5	0.004
20	1-Pentene, 4-methyl	691-37-2	0.15
21	Cyclopentane	287-92-3	0.05
22	Pentane, 2-methyl	107-83-5	0.69
23	C6-alkene		0.03
24	Furan, 2,5-dihydro	1708-29-8	0.02
25	1-Hexene	592-41-6	0.01
26	C6-alkene		0.003
27	Pentane, 3-methyl	96-14-0	0.14
28	1-Pentene, 2-methyl	763-29-1	0.06

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
29	C6-alkene		0.21
30	3-Buten-2-one	78-94-4	0.02
31	2-Butanone	78-84-2	0.17
32	3-Hexene, (Z)	7642-09-3	0.02
33	2-Hexene, (Z)	7688-21-3	0.04
34	1-Butene, 2,3-dimethyl	563-78-0	0.03
35	Cyclopropane, 1,2-dimethyl-3-methylene	4866-55-1	0.02
36	Cyclopropane, propyl	2415-72-7	0.03
37	C6-alkene and others		0.02
38	Cyclopropane, (1-methylethyl)-	3638-35-5	0.08
39	2-Propanol	67-63-0	0.30
40	Furan, tetrahydro	109-99-9	0.25
41	1,3-Pentadiene, 2-methyl	1118-58-7	0.05
42	1,4-Hexadiene	592-45-0	0.03
43	Cyclopropane, butyl	930-57-4	0.02
44	C4-Cyclopropane		0.009
45	2-Butenal	4170-30-3	0.04
46	2-Butanone, 3-methyl-	563-80-4	0.003
47	Hexane, 2-methyl	591-76-4	0.06
48	1,4-Hexadiene	592-45-0	0.001
49	1-Hexene, 3,4-dimethyl	16745-94-1	0.003
50	Cyclohexene	110-83-8	0.004
51	Cyclopropane, butyl	930-57-4	0.01
52	Cyclopropane, butyl	930-57-4	0.01
53	Cyclobutane, isopropyl		0.01
54	Cyclopropane, butyl	930-57-4	0.09
55	3-Heptene, (E)	14686-14-7	0.004
56	2-Butanol	78-92-2	0.001
57	2-Heptene	592-77-8	0.01

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
58	Pentane, 2,4-dimethyl	108-08-7	0.01
59	2-Heptene	592-77-8	0.01
60	Cyclohexane, methyl	108-87-2	0.05
61	C7-alkene		0.001
62	Hexane, 2,4-dimethyl	589-43-5	0.002
63	Cyclopentane, ethyl	1640-89-7	0.01
64	2-Pentanol, 2-methyl	590-36-3	0.01
65	Cyclopentane, 1,2,4-trimethyl	4850-28-6	0.01
66	2-Pentanone, 4-methyl	108-10-1	0.01
67	1-Heptene, 3-methyl- and others	4810-09-7	0.001
68	Mixture		0.01
69	C8-alkene		0.03
70	1-Octene	111-66-0	0.002
71	Hexane, 2,3-dimethyl	584-94-1	0.03
72	Mixture		0.02
73	Heptane, 3-methyl	589-81-1	0.04
74	Cyclohexane, 1,3-dimethyl	638-04-0	0.01
75	2,4-Hexadiene, 3-methyl- and C2-Cyclohexane	28823-42-9	0.004
76	Unknown		0.001
77	3-Hexanone	589-38-8	0.02
78	Alkene		0.004
79	C7-Alkene		0.01
80	Ethane, 1,2-dimethoxy	110-71-4	0.003
81	4-Octene, (E)	14850-23-8	0.01
82	Ethene, tetrachloro	127-18-4	0.001
83	Acetic acid, butyl ester	123-86-4	0.01
84	Hexamethylcyclotrisiloxane	541-05-9	0.01
85	Alkene		0.001
86	Pyridine, 3-methyl	108-99-6	0.004

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
87	Heptane, 2,6-dimethyl	1072-05-5	0.03
88	4-Heptenal, (Z)	6728-31-0	0.01
89	Cyclohexane, ethyl	1678-91-7	0.02
90	Cyclohexane, 1,1,3-trimethyl	3073-66-3	0.02
91	Alkanol and alkene		0.01
92	Mixture		0.01
93	Mixture		0.01
94	Cyclohexane, 1,3,5-trimethyl	1839-63-0	0.01
95	Heptane, 2,3-dimethyl	3074-71-3	0.01
96	Octane, 4-methyl	2216-34-4	0.03
97	Octane, 3-methyl	2216-33-3	0.04
98	4-Heptanone	123-19-3	0.02
99	Benzene, 1,2-dimethyl	95-47-6	0.01
100	Heptane, 2,5-dimethyl	2216-30-0	0.02
101	Butane, 1,1'-oxybis	142-96-1	0.01
102	3-Heptanone	106-35-4	0.05
103	Styrene	100-42-5	0.01
104	3-Heptanol	589-82-2	0.01
105	Heptanal and others	111-71-7	0.01
106	1-Hexene, 3,5,5-trimethyl-	4316-65-8	0.002
107	1,1,2,3-Tetramethylcyclohexane		0.001
108	1R,2T,4C,5T-1,2,4,5-Tetramethylcyclohexane		0.001
109	Cyclohexane, 1-ethyl-4-methyl, trans	6236-88-0	0.01
110	2-Heptanone, 3-methyl	2371-19-9	0.01
111	Mixture		0.02
112	2-Heptanol, 2-methyl and others		0.002
113	Octane, 2,6-dimethyl	2051-30-1	0.03
114	Cyclohexane, 1-propenyl	5364-83-0	0.003
115	Pyridine, 3,5-dimethyl and others	591-22-0	0.01

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
116	Heptane, 3-ethyl-2-methyl	14676-29-0	0.01
117	C9-alkene		0.01
118	2-Heptanone, 6-methyl	928-68-7	0.05
119	Octane, 3,4-dimethyl	15869-92-8	0.01
120	Benzene, propyl-	103-65-1	0.00
121	Nonane, 4-methyl	17301-94-9	0.01
122	1,1,2,3-tetramethylcyclohexane		0.03
123	C3-benzene and alkane		0.02
124	Octane, 2,3,7-trimethyl	62016-34-6	0.02
125	Cycloheptane, methoxy and others		0.005
126	Alkyl-cyclohexene		0.002
127	Cyclohexane, 1-methyl-4-(1-methylethyl)	6069-98-3	0.01
128	C4-Cyclohexane		0.001
129	Cyclohexane, 1-methyl-4-(1-methylethyl)	6069-98-3	0.005
130	Phenol	105-95-2	0.01
131	Cyclotetrasiloxane and C4-cyclohexane		0.02
132	Butanoic acid butyl ester	109-21-7	0.01
133	Decane	124-18-5	0.06
134	Cyclopentane, (2-methylbutyl)-	53366-38-4	0.001
135	Cyclohexane, 1-methyl-3-propyl	4291-80-9	0.01
136	3-Hexene, 3-ethyl-2,5-dimethyl	62338-08-3	0.004
137	Cyclooctane, 1,5-dimethyl	21328-57-4	0.01
138	1-Octanol, 2 butyl and others		0.005
139	3-Hexene, 2,2,5,5-tetramethyl and others		0.01
140	Nonane, 2,6-dimethyl	17302-28-2	0.04
141	Mixture		0.005
142	1-Hexanol, 2-ethyl	104-76-7	0.01
143	Mixture		0.01
144	C5-Cyclohexane		0.02

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
145	C5-Cyclohexane		0.003
146	Cyclopropane, 1,1,2-trimethyl-3-(2-methy	41977-43-9	0.01
147	Nonane, 4,5-dimethyl	17302-23-7	0.01
148	1,1-Dimethyl-2-propylcyclohexane		0.02
149	Decane, 4-methyl	2847-72-5	0.01
150	Decane, 2-methyl	6975-98-0	0.02
151	Naphthalene, decahydro, trans	493-02-7	0.03
152	Ethanone, 1-phenyl	98-86-2	0.01
153	Phenol, 3-methyl	108-39-4	0.01
154	Cyclohexane, 1-(cyclohexylmethyl)-4-met	54823-98-2	0.01
155	Cyclohexane, 2,4-diethyl-1-methyl	61142-70-9	0.004
156	5-Undecene	4941-53-1	0.02
157	2-Nonanone	821-55-6	0.005
158	Benzenemethanol, a,a-dimethyl-	617-94-7	0.01
159	Undecane	1120-21-4	0.09
160	5-Undecene	4941-53-1	0.003
161	Furan, 3-(1,1-dimethylethyl)2,3-dihydro	34314-82-4	0.004
162	Cyclopropane, 1-butyl-1-methyl-2-propyl	41977-34-8	0.005
163	Undecane, 5-methyl	1632-70-8	0.02
164	1-Nonyne	3452-09-3	0.01
165	Butanoic acid, 2-hexenyl ester, (E)	53398-83-7	0.04
166	3-Decyne	2384-85-2	0.003
167	6-Dodecene, (E)	7206-17-9	0.01
168	Cyclohexane, pentyl	4292-92-6	0.02
169	Naphthalene, decahydro-2-methyl	2958-76-1	0.03
170	1-Undecene, 4-methyl	74630-39-0	0.004
171	6-Methylundecane	17302-33-9	0.04
172	Undecane, 4-methyl	2980-69-0	0.02
173	Undecane, 2-methyl	7045-71-8	0.03

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
174	C11-alkene		0.01
175	Undecane, 3-methyl	1002-43-3	0.01
176	C2-decahydronaphthalene		0.003
177	3-Undecene, 8-methyl		0.01
178	Naphthalene, decahydro, 1,5-dimethyl	66552-62-3	0.004
179	Decane, 2,3,6-trimethyl	62238-12-4	0.01
180	C13-alkene		0.002
181	Cyclohexane, 1-methyl-3-pentyl	54411-02-8	0.01
182	Cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	0.01
183	Undecane, 2,4-dimethyl and others		0.002
184	Undecane, 2,6-dimethyl	17301-23-4	0.07
185	Alkenyl-cyclopentane		0.004
186	Nonane, 5-butyl	17312-63-9	0.01
187	Undecane, 3-methyl	1002-43-3	0.003
188	Cyclopentane, 1,1,3-trimethyl-3-(2-meth	74421-09-3	0.01
189	Cyclopentane, 1-pentyl-2-propyl	62199-51-3	0.003
190	Alkene		0.001
191	Cyclohexane, 2-butyl-1,1,3-trimethyl	54676-39-0	0.02
192	C3-decahydronaphthalene		0.002
193	C3-decahydronaphthalene		0.01
194	C3-decahydro-naphthalene		0.01
195	Cyclohexane, hexyl	4292-75-5	0.02
196	Dodecane, 6-methyl	6044-71-9	0.01
197	Undecane, 2,4-dimethyl	17312-80-0	0.01
198	Dodecane, 4-methyl	6117-97-1	0.02
199	Undecane, 2,10-dimethyl	17301-27-8	0.04
200	Decane, 2,6,7-trimethyl	62108-25-2	0.12
201	C7-cyclohexane		0.03
202	2(3H)-Benzofuranone,3a,4,5,6-tetrahydr	16778-26-0	0.01

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
203	1-Tridecene	2437-56-1	0.003
204	6-Tetradecene, cis		0.04
205	Phenol, 4-(1,1-dimethylethyl)- and others		0.01
206	Undecnae, 2,4-dimehtyl	17312-80-0	0.005
207	C14-alkane		0.01
208	Tridecane, 6-methyl	13287-21-3	0.03
209	1-Dodecanol	112-53-8	0.001
210	C8-Cyclohexane		0.01
211	C8-Cyclohexane		0.001
212	Mixture		0.001
213	Mixture		0.01
214	C9-cyclopentane		0.01
215	Tetradecane	629-59-4	0.02
216	Cyclohexane, octyl	1795-15-9	0.04
217	Tridecane, 4-methyl	26730-12-1	0.02
218	Tridecane, 2-methyl	1560-96-9	0.03
219	Alkane		0.004
220	Decane, 2,3,8-trimethyl-	62238-14-6	0.002
221	Tridecane, 3-methyl	6418-41-3	0.05
222	Dodecane, 2,6,10-trimethyl	3891-98-3	0.15
223	Tetradecane	629-59-4	0.15
224	Tridecane, 4,8-dimethyl	55030-62-1	0.03
225	Cyclohexane, 1,1,3-trimethyl-2-(3-methy	54965-05-8	0.01
226	Dodecane, 2,6,11-trimethyl	31295-56-4	0.02
227	Alkanol		0.01
228	Dodecane, 2,6,11-trimethyl	31295-56-4	0.02
229	C15-Alkane		0.01
230	Dodecane, 2,6,11-trimethyl or C15-alkane		0.03
231	Hexadecane	544-76-3	0.16

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
232	Tetradecane, 3-methyl	18435-22-8	0.02
233	Alkane		0.01
234	C16-alkane		0.02
235	1-Hexadecene	629-73-2	0.03
236	Pentadecane	629-62-9	0.14
237	1-Tetradecanol	112-72-1	0.002
238	C9-Cyclopentane		0.002
239	C9-Cyclohexane		0.01
240	C7-Cyclohexane		0.01
241	Tridecane, 5-propyl	55045-11-9	0.002
242	Tetradecane, 2,6,10-trimethyl	14905-56-7	0.02
243	Tetradecane, 4,11-dimethyl	55045-12-0	0.005
244	Dodecane, 2-methyl-8-propyl	55045-07-3	0.01
245	Decane, 3-cyclohexyl, 3-cyclohexyl	13151-74-1	0.02
246	Hexadecane, 2-methyl	1560-92-5	0.01
247	5-Undecanone, 2-methyl	50639-02-6	0.005
248	Pentadecane	629-62-9	0.004
249	Hexadecane	544-76-9	0.05
250	3-Hexadecene, (Z)-	34303-81-6	0.001
251	Propanoic acid, 2-methyl,1-(1,1-dimeth	74381-40-1	0.03
252	1,2-Benzenedicarboxylic acid, diethyl ester	84-66-2	0.01
253	Pentadecane, 2,6,10-trimethyl		0.01
254	Cyclohexane, decyl	1795-16-0	0.002
255	5-Undecanone, 2-methyl	50639-02-6	0.002
256	1-Hexadecene	629-73-2	0.005
257	Heptadecane	629-78-7	0.01
258	Pentadecane, 2,6,10,14-tetremethyl	1921-70-6	0.01
259	Tetradecanoic acid	544-63-8	0.01
260	Octadecane	593-45-3	0.001

Cmpd #	Compound	CAS[1] Number	Average[2] (mg/m^3)
261	Siloxane		0.001
262	Benzenesulfonamide, N-butyl	3622-84-2	0.03
263	2-Pentadecanone, 6,10,14-trimethyl	502-69-2	0.003
264	Pentadecanoic acid	1002-84-2	0.001
265	1-Hexadecanol	36653-82-4	0.002
266	Hexanedioic acid, dioctyl ester	123-79-5	0.002
267	Mixture		0.001
268	2-Heptadecanone	2922-51-2	0.000
269	2-Pentadecanone, 6,10,14-trimethyl	502-69-2	0.001
270	Hexadecanoic acid	57-10-3	0.01
271	Hexadecane, 2,6,10,14-tetramethyl	638-36-8	0.001
272	Hexadecanoic acid, 1-methylethyl ester	142-91-6	0.004

1. CAS = Chemical Abstract Service.

2. Average includes samples where concentration was zero.

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