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Tank 241-BY-107 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-421)		ECN No.

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Page 1 of 1

1. EDT 607555

2. To: (Receiving Organization)	3. From: (Originating Organization)	4. Related EDT No.:
Distribution	Tank Vapor Characterization Program	N/A
5. Proj./Prog./Dept./Div.:	**6. Cog. Engr.:**	**7. Purchase Order No.:**
Characterization	J. W. Osborne	N/A
8. Originator Remarks: N/A		**9. Equip./Component No.:** N/A
		10. System/Bldg./Facility: N/A
11. Receiver Remarks: N/A		**12. Major Assm. Dwg. No.:** N/A
		13. Permit/Permit Application No.: N/A
		14. Required Response Date: N/A

15. DATA TRANSMITTED

(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	(F) Approval Designator	(G) Reason for Transmittal	(H) Originator Disposition	(I) Receiver Disposition
1	WHC-SD-WM-ER-421	N/A	0	Tank 241-BY-107 Vapor Sampling and Analysis Tank Characterization Report	N/A	2	1	1

16. KEY

Approval Designator (F)	Reason for Transmittal (G)	Disposition (H) & (I)
E, S, Q, D or N/A (see WHC-CM-3-5, Sec.12.7)	1. Approval 4. Review 2. Release 5. Post-Review 3. Information 6. Dist. (Receipt Acknow. Required)	1. Approved 4. Reviewed no/comment 2. Approved w/comment 5. Reviewed w/comment 3. Disapproved w/comment 6. Receipt acknowledged

17. SIGNATURE/DISTRIBUTION
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Document Number:	WHC-SD-WM-ER-421, REV 0
Document Title:	Tank 241-BY-107 Vapor Sampling and Analysis Tank Characterization Report
Release Date:	5/9/95

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

APPROVED FOR PUBLIC RELEASE

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SUPPORTING DOCUMENT

1. Total Pages 28

2. Title	3. Number	4. Rev No.
Tank 241-BY-107 Vapor Sampling and Analysis Tank Characterization Report	WHC-SD-WM-ER-421	0

5. Key Words	6. Author
241-BY-107, headspace vapor samples, organic analytes, VSS, SUMMA™, inorganic gases and vapors	Name: J. L. Huckaby Signature Organization/Charge Code Tank Vapor Characterization Program/N4AB1/W75600

7. Abstract

Tank 241-BY-107 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-107 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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TANK 241-BY-107 VAPOR SAMPLING AND ANALYSIS TCR CHAPTER

X.0 HEADSPACE GAS AND VAPOR SAMPLES

Tank BY-107 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-107 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

Tank BY-107 was vapor sampled in March 1994 using the *in situ* sampling (ISS) method, and again in October 1994 using the more robust vapor sampling system (VSS) method. There were problems with the March 1994 sampling event (i.e., some samples were radiolytically contaminated) and only the SUMMA™ canister samples were analyzed. Nearly all of results presented here are from the October 1994 sampling event.

X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank BY-107 using the vapor sampling system (VSS) on October 26, 1994 by WHC Sampling & Mobile Laboratories (S&ML), (WHC 1995). Sample collection and analysis were performed as directed by the tank characterization plan (Carpenter 1994). The tank headspace temperature was determined to be 33.1 °C. Air from the tank BY-107 headspace was withdrawn via a 5.5 m-long heated sampling probe mounted in riser 5, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C. Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL).

The 40 tank air samples and 2 ambient air control samples collected are listed in Table X-1 by analytical laboratory. Table X-1 also lists the 14 trip blanks and 2 field blanks that accompanied the samples. A general description of vapor sampling and sample analysis methods is given by Huckaby (1994). 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

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

million by volume (ppmv). Inorganic analyte sorbent traps and SUMMA™ canisters were prepared and analyzed by PNL. Ligotke et al. (1995) describe sample preparation and analyses.

The relative standard deviations of the results, given in the last column in Table X-2, indicate the precision of reported results is good. Relative standard deviations range from 0.6 % for ammonia, to 28 % for carbon dioxide 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 relative standard deviations suggest there were no significant problems in the field or in the laboratories.

X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 972 ppmv, is among the highest observed to date in the waste tanks, and is about 39 times the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1990).

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 267 ppmv of hydrogen in tank BY-107, 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-107, 621 ppmv, is about 25 times the NIOSH 8-hr REL of 25 ppmv (NIOSH 1976, 1977).

For comparison, the measured concentrations of ammonia, hydrogen, and nitrous oxide for tanks BY-104, BY-105, BY-106, BY-107, and BY-108 are given in Table X-3.

X.2.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 94 ppmv, is about one-fourth of the normal ambient air concentration of about 400 ppmv. Lower than ambient carbon dioxide concentrations are expected in the waste tank headspaces. 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. The 94 ppmv carbon dioxide concentration measured in tank BY-107 is typical of other tanks sampled to date.

Carbon monoxide in the tank BY-107 headspace, measured to be < 20 ppmv, is below the NIOSH 8-hr REL of 35 ppmv. Its concentration in ambient air

typically ranges from 0.05 to 0.15 ppmv. Elevated waste tank headspace carbon monoxide concentrations are common, and have been measured to be as high as 26.7 ppmv in tank C-103 (Huckaby and Story 1994). Elevated carbon monoxide concentrations are thought to be due to the decomposition of organic waste in the tanks.

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

Nitric oxide and nitrogen dioxide concentrations in the tank BY-107 headspace were determined to be 0.13 ppmv and $\leq$ 0.02 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-107. 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-107 was determined to be about 13.0 mg/L, at the tank headspace temperature of 33.1 °C and pressure of 981 mbar (735.7 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 18.31 mbar (13.7 torr), to a dew point of 16.1 °C, and to a relative humidity of 36 %.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium ions 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-107 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. (1995). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method (EPA 1988) was also performed by Oregon Graduate Institute of Science and Technology (OGIST) on samples collected in March 1994 by the ISS method (Pingel 1994, Rasmussen 1994a).

X.3.1 Positively Identified Organic Analytes

ORNL positively identified 24 of 27 target analytes selected by WHC. Three target analytes, vinylidene chloride, tributyl phosphate, and dibutyl butylphosphonate, were below detection limits. The detected analytes, and their average concentrations from the analysis of 3 TSTs, are given in Table X-4. The 27 TST target analytes for tank BY-107 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). Five of the target analytes were measured to be above the method's upper calibration limit. Two of the target analytes, dichloromethane and heptanenitrile, were positively identified by ORNL, but below the method quantitation limit.

Also given in Table X-4 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL. PNL performed analyses according to the EPA task order 14 (TO-14) methodology, but expanded the number of target analytes from 40 to 54 to include waste tank analytes of particular interest (EPA 1988, Clauss et al. 1995). Of the original 40 TO-14 analytes, 37 were determined to be below the 0.002 ppmv quantitation limit of the analyses (Clauss et al. 1995 provide the complete TO-14 analyte list), and 4 of the 14 additional target analytes (acetonitrile, pyridine, butanenitrile, and propanenitrile) were below the 0.005 ppmv method quantitation limit. Averages reported are from analyses of 3 SUMMA™ canister samples.

Ten target analytes were common to both the ORNL and PNL analyses. Comparison of the results from the 2 laboratories indicates the following:

1) An acceptable agreement for the nonpolar analytes (i.e., n-hexane, benzene, n-heptane, toluene, and n-decane) and acetone;

2) a significant disagreement regarding the existence of nitriles. Specifically, TST analyses indicate acetonitrile at 2.2 ppmv, propanenitrile at 0.047 ppmv, butanenitrile at 0.12 ppmv, and pentanenitrile at 0.028 ppmv, while SUMMA™ analyses indicate each of these to be below their quantitation limits 0.005 ppmv.

That the nitriles observed in TST samples were not detected in SUMMA™ canister samples indicates there may have been a problem with the SUMMA™ analyses. There would not appear to be any fundamental problem with recovering nitriles from SUMMA™ canisters, because nitriles have been observed in SUMMA™ samples from other waste tanks, in concentrations that agree with TST results. While it is also possible that TST samples were contaminated with the nitriles, it appears more likely that the nitriles were present in the tank headspace.

The most abundant analytes in Table X-4 are 1-butanol, acetone, acetonitrile, 1-propanol, and 2-butanone. Each of these was measured to be above 1 ppmv. At the reported concentrations, the Table X-4 analytes do not individually or cumulatively represent a flammability hazard.

X.3.2 Tentatively Identified Organic Analytes

In addition to targeted analytes, both ORNL and PNL analytical procedures allow the tentative identification of other organic vapors. By the nature of the samples and their analysis, virtually all 3 to 15 carbon organic compounds present in the tank headspace above analytical detection limits are observable. The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table X-5, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table X-6. Estimated concentrations are in mg/m^3, based on dry air at 0 °C and 1.01 bar.

Both ORNL and PNL tentatively identify analytes by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and also determines its molecular weight (which specifies the number of carbon atoms in the molecule). The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Entries in Table X-6, particularly near the bottom of the table where the analytes have higher molecular weights, illustrate this.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Clauss et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-5 and X-6 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 80 and 81 in Table X-6). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

Concentrations given in Tables X-5 and X-6 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

X.3.3 Total Nonmethane Organic Compounds

OGIST measured the total nonmethane organic compound (TNMOC) concentration in 3 SUMMA™ canister samples using the EPA TO-12 method (Rasmussen 1994a). The sample mean was 173 mg/m^3, with a standard deviation of 6 mg/m^3. Though data on other tanks is very limited, this value is high compared to other waste tanks sampled to date. For comparison, the TNMOC concentration in clean ambient air may range from 0.03 to 0.1 mg/m^3, in polluted city air it may be 0.3 to 0.4 mg/m^3, tank C-103 has an estimated 3,000 to 5,000 mg/m^3 (Rasmussen and Einfeld 1994), and tank BY-106 has about 9.9 mg/m^3 (Rasmussen 1994b).

The sum of the ORNL target analyte concentrations, 55.2 mg/m^3, and the ORNL estimated concentrations of tentatively identified analytes, 93.9 mg/m^3, is

149.1 mg/m^3. This value is in very good agreement (given method differences) with the EPA TO-12 value of 173 mg/m^3.

X.3.4 Discussion of Organic Analytes

In general, the organic analytes observed in the waste tank headspaces are indicative of the types of volatile and semivolatile organic waste that resides in each tank. Examination of the data provides clues to both the current organic constituents and the chemical reactions that are taking place.

Some of the compounds listed in Tables X-4, X-5, and X-6 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane, n-tridecane, n-tetradecane, n-pentadecane) and methyl-substituted decahydronaphthalenes that were used as diluents for tributyl phosphate.

Most of the compounds in Tables X-4, X-5, and X-6 are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. For example, 1-butanol is known to be formed by the hydrolysis of tributyl phosphate, and it has been suggested that the alcohols, aldehydes, ketones, nitriles, alkenes, and short chain alkanes are all degradation products of the semivolatile NPHs.

In the semivolatile region of Tables X-5 and X-6, there are many branched alkanes. The abundance of these, as well as the decahydronaphthalenes, may indicate the origin of the tributyl phosphate diluent presently in tank BY-107.

Though their concentrations are not significant many alcohols were tentatively identified by PNL and ORNL (Table X-6). These have generally not been observed to be as numerous in other NPH-rich tank headspaces, which tend to be dominated by aldehydes, ketones, alkanes, and alkenes.

Table X-1
Tank BY-107 Gas and Vapor Sample Type and Number

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.05, 0.25 and 0.5	Organic vapors	12 tank air samples + 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample

Table X-2
Tank BY-107 Inorganic Gas and Vapor Concentrations

Compound	CAS[1] Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
Ammonia, NH_3	7664-41-7	Sorbent Trap	6	972	6	0.6
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	94	26	28
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 20	--	--
Hydrogen, H_2	1333-74-0	SUMMA™	3	267	36	14
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.13	0.03	23
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	621	36	6
Water Vapor, H_2O	7732-18-5	Sorbent Trap	6	18,700 (13.0 mg/L)	600 (0.4 mg/L)	3

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

Table X-3
Comparison of Selected Analytes
in Tanks BY-104, BY-105, BY-106, BY-107 and BY-108

Tank	Ammonia (ppmv)	Hydrogen (ppmv)	Nitrous Oxide (ppmv)	TNMOC[1] (mg/m^3)
BY-104[2]	248	295	201	60.8
BY-105[3]	43	48	50	12.7
BY-106[4]	74	46	71	9.9
BY-107[5]	972	267	621	173
BY-108[6]	1040	399	641	594

1. TNMOC = total nonmethane organic compounds.

2. Ammonia result is from Clauss et al. 1994; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994b.

3. Ammonia result is from Pool et al. 1995; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994c.

4. Ammonia result is from Lucke et al. 1995; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994d.

5. Ammonia, hydrogen, and nitrous oxide results are from Clauss et al. 1995; TNMOC result is from Rasmussen 1994a.

6. Ammonia, hydrogen, and nitrous oxide results are from McVeety et al. 1995; TNMOC result is from Rasmussen 1994a.

Table X-4
Tank BY-107 Organic Target Compound Average Concentrations

Compound	CAS[1] Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
Trichlorofluoromethane	75-69-4	SUMMA™,[3]	0.030	0.002	7
Acetonitrile[4]	75-05-8	TST[5]	2.2	0.9	40
		SUMMA™	< 0.005	--	--
Propanone (acetone)[4]	67-64-1	TST	3.9	2.2	57
		SUMMA™	6.5	0.7	10
1-Propanol	71-23-8	SUMMA™	1.8	0.2	14
Dichloromethane[4]	75-09-2	TST	0.012	0.007	54
Propanenitrile	107-12-0	TST	0.047	0.012	25
		SUMMA™	< 0.005	--	--
Butanal[4]	123-72-8	TST	0.13	0.20	153
2-Butanone	78-93-3	SUMMA™	1.1	0.03	3
n-Hexane[4]	110-54-3	TST	0.94	0.12	13
		SUMMA™	0.79	0.07	9
Benzene	71-43-2	TST	0.037	0.006	16
		SUMMA™	0.0048	0.0003	6
1-Butanol[4]	71-36-3	TST	7.9	5.0	63
Butanenitrile	109-74-0	TST	0.12	0.08	68
		SUMMA™	< 0.005	--	--
2-Pentanone	107-87-9	TST	0.23	0.12	53
4-Methyl-2-pentanone	108-10-1	SUMMA™	0.028	0.003	12

Cyclohexane	110-82-7	SUMMA™	0.078	0.048	62
n-Heptane	142-82-5	TST	0.35	0.12	34
		SUMMA™	0.19	0.01	5
Tetrahydrofuran	109-99-9	SUMMA™	0.56	0.01	1
Toluene	108-88-3	TST	0.067	0.007	11
		SUMMA™	0.036	0.002	7
Cyclohexanone	108-94-1	SUMMA™	0.0059	0.0022	38
Pentanenitrile	110-59-8	TST	0.028	0.002	6
		SUMMA™	< 0.005	--	--
2-Hexanone	591-78-6	TST	0.15	0.03	17
n-Octane	111-65-9	TST	0.12	0.02	13
Hexanenitrile	628-73-9	TST	0.018	0.002	9
2-Heptanone	110-43-0	TST	0.12	0.02	19
n-Nonane	111-84-2	TST	0.066	0.005	8
Heptanenitrile[4]	629-08-3	TST	0.013	0.002	18
2-Octanone	111-13-7	TST	0.035	0.005	13
n-Decane	124-18-5	TST	0.068	0.010	14
		SUMMA™	0.033	0.003	9
n-Undecane	1120-21-4	TST	0.14	0.004	3
n-Dodecane	112-40-3	TST	0.21	0.001	0.5
n-Tridecane	629-50-5	TST	0.26	0.01	4
Sum of positively identified compounds:			23.5		

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. SUMMA™ canister results based on analyses of 3 samples.
4. Two or more samples fell outside of calibration range.
5. TST results are based on analyses of 3 samples.

Table X-5
Tank BY-107 Tentatively Identified Organic Compounds in SUMMA™ Samples

Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
Propane	74-98-6	0.81	0.33
Propene	115-07-1	1.01	0.22
Cyclopropane	75-19-4	0.19	0.01
Isobutane	75-28-5	0.34	0.02
1-Butene	106-98-9	0.36	0.02
n-Butane	106-97-8	0.85	0.04
1-Propene, 2-methyl-	115-11-7	0.17	0.01
Isopropyl Alcohol	67-63-0	0.30	0.01
n-Pentane	109-66-0	0.55	0.00
2-Methylpentane	107-83-5	0.76	0.01
3-Methylpentane	96-14-0	0.15	0.00
2-Butanol	78-92-2	0.13	0.00
Methylcyclopentane	96-37-7	0.09	0.00
3-methyl-2-Butanone	563-80-4	0.12	0.00
1-Butanol	71-36-3	2.66	0.27
2-Pentanone	107-87-9	0.91	0.07
Hexane, 3-methyl-	589-34-4	0.53	0.01
2-Pentanol	6032-29-7	0.09	0.00
1-Heptene	592-76-7	0.08	0.00
C7 Alkene/Cycloalkane		0.07	0.00
2-Methyl-2-Pentanol	590-36-3	0.10	0.00
Methylcyclohexane	108-87-2	0.17	0.00
1-Pentanol	71-41-0	0.08	0.00
2-Methylheptane	592-27-8	0.30	0.01
2-Hexanone	591-78-6	0.31	0.01
n-Octane	111-65-9	0.29	0.01
Alkane		0.13	0.01

1,1,3-Trimethylcyclohexane	3073-66-3	0.11	0.01
3-Heptanone	106-35-4	0.22	0.01
2-Heptanone	110-43-0	0.23	0.00
n-Nonane	111-84-2	0.20	0.01
2-Heptanone, 6-methyl-	928-68-7	0.38	0.01
C3 substituted Cyclohexane		0.07	0.00
2-Octanone	111-13-7	0.10	0.00
C4 substituted Cyclohexane		0.09	0.00
C11 Alkane		0.22	0.01
C4 substituted Cyclohexane		0.16	0.03
C11 Alkane		0.07	0.00
n-Undecane	1120-21-4	0.71	0.02
Methyldecahydronaphthalene		0.11	0.02
Cyclohexane, pentyl-	4292-92-6	0.15	0.01
C12 Alkane		0.11	0.00
C12 Alkane		0.17	0.01
n-Dodecane	112-40-3	1.47	0.05
Decahydro-2,6-Dimethylnaphtalene	1618-22-0	0.09	0.00
C13 Alkane		0.90	0.04
Decahydro-2,3-Dimethylnaphthalene	1008-80-6	0.11	0.01
C7 substituted Cyclohexane		0.49	0.02
Unknown		0.16	0.01
Alkane		0.26	0.02
Alkane		0.17	0.01
Alkane		1.37	0.10
n-Tridecane	629-50-5	1.98	0.17
Alkene/Cycloalkane		0.08	0.01
Alkene/Cycloalkane		0.26	0.02
Alkane		0.30	0.02
Alkene/Cycloalkane		0.32	0.03
2-methyltridecane	1560-96-9	0.20	0.02

3-Methyltridecane	6418-41-3	0.11	0.01
C15 Alkane		1.20	0.10
n-Tetradecane	629-59-4	1.12	0.07
Alkene/Cycloalkane		0.13	0.01
Alkane		0.20	0.00
Sum of tentatively identified compounds:		25.57	

1. CAS = Chemical Abstract Service.

Table X-6
Tank BY-107 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
1	1-propene, 2-methyl-	115-11-7	1.0	0.1
2	cyclopropane, 1,1-dimethyl	1630-94-0	0.17	0.29
3	cyclobutane	287-23-0	0.15	0.26
4	butane, 2-methyl-	78-78-4	3.1	0.8
5	cyclopropane, ethyl-	1191-96-4	4.0	4.9
6	2-propanol	67-63-0	2.1	1.9
7	cyclopropane, ethyl-	1191-96-4	0.67	0.15
8	1-hexene	592-41-6	0.69	0.21
9	cyclopentane	287-92-3	0.43	0.38
10	pentane, 2-methyl-	107-83-5	6.9	1.6
11	1-propene, 2-fluoro-	1184-60-7	1.0	0.3
12	pentane, 3-methyl-	96-14-0	1.2	0.3
13	1-pentene, 2-methyl-	763-29-1	0.12	0.21
14	1-hexene	592-41-6	0.61	0.16
15	2-butanone	78-93-3	1.0	1.7
16	2-butanol	78-92-2	0.45	0.45
17	cyclopropane, propyl-	2415-72-7	0.53	0.28
18	cyclobutane, ethyl-	4806-61-5	0.19	0.33
19	1-pentene-2-methyl	763-29-1	0.29	0.50
20	furan, tetrahydro-	109-99-9	2.0	0.4
21	1,3-pentadiene, 2-methyl-	1118-58-7	0.14	0.24
22	hexane, 2-methyl-	591-76-4	0.61	0.20
23	alkanone		0.091	0.158
24	2-pentanol	6032-29-7	0.55	0.28
25	cyclohexane, methyl-	108-87-2	0.51	0.24
26	2-pentanol, 2-methyl-	590-36-3	0.078	0.135
27	2-pentanone, 4-methyl-	108-10-1	0.31	0.11

28	1-heptene, 6-methyl-	5026-76-6	0.054	0.094
29	hexane, 2,3-dimethyl	584-94-1	0.70	0.67
30	furan, 2,5-dihydro	1708-29-8	0.75	1.30
31	2(3H)-furanone, dihydro-3,5-dimethyl-	5145-01-7	0.17	0.30
32	3-pentanol, 2-methyl-	565-67-3	0.051	0.089
33	hexanal, 3-methyl-	19269-28-4	0.18	0.30
34	2-pentene, (E)-	646-04-8	0.24	0.41
35	3-hexanone	589-38-8	0.30	0.06
36	2-octanol	123-96-6	0.14	0.24
37	propane, 2,2'-oxybis	108-20-3	0.15	0.25
38	methylamine, N-(1-methylbutylidene)-	22431-09-0	0.39	0.41
39	2-heptanol	543-49-7	0.092	0.159
40	tetrachloroethene	127-18-4	0.26	0.45
41	acetic acid, butyl ester	123-86-4	0.19	0.17
42	1,4-butanediol, dinitrate	3457-91-8	0.048	0.083
43	heptane, 2,6-dimethyl-	1072-05-5	0.29	0.09
44	cyclohexane, ethyl-	1678-91-7	0.24	0.09
45	cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.67	0.46
46	1-hexene, 3,4-dimethyl-	16745-94-1	0.34	0.27
47	hexane, 3-methoxy-	54658-01-4	0.24	0.14
48	3-octanone	106-68-3	0.052	0.090
49	heptane, 2,3-dimethyl	3074-71-3	0.040	0.070
50	octane, 2-methyl- and c2-benzene	3221-61-2	0.17	0.18
51	octane, 3-methyl- and c2-benzene	2216-33-3	0.17	0.29
52	benzene, ethyl and alkane	71-43-2	0.056	0.097
53	hexane, 2,2,3-trimethyl and c2-benzene		0.54	0.54
54	4-heptanone	123-19-3	0.13	0.01
55	unknown		0.042	0.073

56	3-heptanone	106-35-4	0.57	0.07
57	3-heptanol	589-82-2	0.31	0.22
58	2-heptanol	543-49-7	0.18	0.01
59	bicyclo[2.2.1]heptane	279-23-2	0.19	0.03
60	octane, 2,6-dimethyl-	2051-30-1	0.11	0.19
61	2-heptanone, 4-methyl	6137-06-0	0.033	0.058
62	heptane, 4-(1-methylethyl)-	52896-87-4	0.028	0.048
63	3-pentanone, 2,4-dimethyl-	565-80-0	0.069	0.060
64	3-octanone	106-68-3	0.026	0.044
65	2-heptanone, 6-methyl-	928-68-7	1.0	0.2
66	nonane, 4-methyl-	17301-94-9	0.11	0.10
67	1,1,2,3-tetramethylcyclohexane A		0.27	0.04
68	nonane, 2-methyl	871-83-0	0.042	0.072
69	2-octanol	123-96-6	0.27	0.07
70	3-butene-2-ol	598-32-3	0.67	0.37
71	decadienal		0.099	0.006
72	cyclopentane, 1,2-dimethyl-3-(1-methyleth	489-20-3	0.13	0.11
73	cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	0.037	0.064
74	phenol	108-95-2	0.029	0.050
75	cyclopentane, 1,2-dimethyl-3-(1-methyl ethyl_	489-20-3	0.20	0.17
76	3-hexene, 3-ethyl-2,5-dimethyl-	62338-08-3	0.093	0.160
77	cyclopentane, 2-isopropyl-1,3-dimethyl	32281-85-9	0.092	0.102
78	cyclopentane, (1-methylbutyl)-	4737-43-3	0.079	0.137
79	nonane, 2,6-dimethyl-	17302-28-2	0.75	0.04
80	nonane, 3,7-dimethyl-	17302-32-8	0.028	0.049
81	nonane, 3,7-dimethyl-	17302-32-8	0.048	0.082

82	1-hexanol, 2-ethyl	104-76-7	0.035	0.061
83	alkane		0.022	0.039
84	3-nonyne and others		0.024	0.041
85	cyclohexane, butyl-	1678-93-9	0.23	0.07
86	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.061	0.105
87	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.030	0.051
88	undecane, 5-methyl-	1632-70-8	0.047	0.081
89	cyclohexane, cyclopropyl	32669-86-6	0.061	0.053
90	1,1-dimethyl-2-propylcyclohexane		0.21	0.02
91	decane, 5-methyl-	13151-35-4	0.25	0.03
92	decane, 4-methyl-	2847-72-5	0.22	0.04
93	2-pentanone, 4-methyl-	108-10-1	0.23	0.39
94	octane, 2,3,3-trimethyl		0.47	0.42
95	naphthalene, decahydro-, trans	493-02-7	0.18	0.17
96	decane, 3-methyl-	13151-34-3	0.43	0.22
97	2-furanacetaldehyde, .alpha.-propyl-	31681-26-2	0.14	0.12
98	4-nonanone and others		0.052	0.090
99	formic acid, 2,6-dimethyl-5-hepten-2-ol ester		0.10	0.02
100	4-decene, 3-methyl-	62338-47-0	0.19	0.05
101	4-hepten-3-one, 5-ethyl-2,4-dimethyl	22319-29-5	0.16	0.15
102	5-undecene	4941-53-1	0.36	0.15
103	2-nonanone	821-55-6	0.29	0.05
104	cyclohexane, 1-ethyl-2-propyl-	62238-33-9	0.11	0.03
105	5-undecene	4941-53-1	0.12	0.03
	'-decene, 4-methyl-, (Z)-	74630-30-1	0.043	0.074
	-undecene, 2,5-dimethyl-	49622-16-4	0.030	0.053

108	undecane, 5-methyl-	1632-70-8	0.67	0.24
109	methyl-decahydronaphthalene		0.10	0.01
110	undecane, 2,8-dimethyl-	17301-25-6	0.40	0.49
111	naphthalene, decahydro-2-methyl	2958-76-1	0.35	0.32
112	undecane, 2,8-dimethyl-	17301-25-6	0.43	0.39
113	cyclopentane, 1-butyl-2-propyl-	62199-50-2	0.052	0.091
114	cyclohexane, pentyl-	4292-92-6	0.14	0.23
115	c4-heptadiene		0.29	0.50
116	cyclooctane, ethenyl-	61142-41-4	0.096	0.017
117	1-dodecene	112-41-4	0.026	0.044
118	3-undecene, 2-methyl-, (Z)-	74630-48-1	0.065	0.061
119	naphthalene, decahydro-2-methyl	2958-76-1	0.99	0.91
120	6-methylundecane	17302-33-9	0.97	0.27
121	undecane, 4-methyl-	2980-69-0	0.52	0.11
122	undecane, 2-methyl-	7045-71-8	1.1	0.3
123	decane, 2,3,8-trimethyl-	62238-14-6	0.26	0.08
124	undecane, 3-methyl-	1002-43-3	0.60	0.13
125	2-undecene, 6-methyl-, (E)-	74630-61-8	0.060	0.105
126	decane, 2,6,7-trimethyl-	62108-25-2	0.18	0.17
127	decane, 2,3,6-trimethyl-	62238-12-4	0.18	0.03
128	cyclododecane	294-62-2	0.14	0.24
129	dimethyl-decahydronaphthalene		0.10	0.18
130	cyclotetradecane	295-17-0	0.27	0.23
131	naphthalene, decahydro-1,6-dimethyl	1750-51-2	0.10	0.18
132	cyclohexane, 1-methyl-4-(1-methylbutyl)-		0.13	0.02
133	1,1'-bicyclohexyl	2-51-3	0.015	0.027
134	undecane, 2,4-dimethyl-	17312-80-0	0.048	0.042
135	undecane, 2,6-dimethyl-	17301-23-4	2.0	0.03

136	undecane, 3,7-dimethyl-	17301-29-0	0.20	0.02
137	decane, 2,3,5-trimethyl- and others		0.23	0.06
138	2-undecene, 7-methyl-, cis=trans		0.055	0.048
139	cyclopentane, 1-pentyl-2-propyl-	62199-51-3	0.023	0.040
140	cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.80	0.01
141	undecane, 5-ethyl-	17453-94-0	0.098	0.013
142	naphthalene, decahydro-1,6-dimethyl-	1750-51-2	0.10	0.04
143	dimethyl-decahydronaphthalene		0.076	0.068
144	cyclohexane, hexyl-	4292-75-5	0.67	0.06
145	undecane, 2,6-dimethyl-	17301-23-4	0.21	0.04
146	dodecane, 5-methyl-	17453-93-9	0.21	0.03
147	dodecane, 4-methyl-	6117-97-1	0.58	0.02
148	dodecane, 2-methyl-	1560-97-0	0.72	0.63
149	undecane, 2,10-dimethyl-	17301-27-8	0.34	0.59
150	dodecane, 4,6-dimethyl	61141-72-8	1.2	2.1
151	trimethyl-decahydronaphthalen e		0.14	0.01
152	decane, 2,6,7-trimethyl-	62108-25-2	1.2	2.0
153	dodecane, 4,6-dimethyl	61141-72-8	1.1	2.0
154	trimethyl-decahydronaphthalen e		0.12	0.11
155	cyclopentane, 1-butyl-2-ethyl-	72993-32-9	0.073	0.069
156	6-tridecene, 7-methyl-	24949-42-6	0.48	0.41
157	5-undecene, 7-methyl-, (Z)-	74630-62-9	0.037	0.064
158	3-tetradecene, (E)-	41446-68-8	0.24	0.41
159	c8-cyclopentane		0.13	0.11
160	c14-alkane		0.14	0.12
161	c14-alkane		0.23	0.20

162	tetradecane	629-59-4	0.84	0.55
163	c14-alkane		0.029	0.050
164	3,3,4,4-tetraethylhexane		0.027	0.047
165	undecane, 2,9-dimethyl-	17301-26-7	0.24	0.11
166	tridecane, 6-methyl	13287-21-3	0.38	0.66
167	cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	0.19	0.16
168	tridecanenitrile	629-60-7	0.030	0.052
169	butane, 2-cyclohexyl-3-methyl		0.055	0.095
170	tridecane, 3-methyl	6418-41-3	0.079	0.137
171	1H-pyrrole, 1-pentyl and others		0.032	0.056
172	c5-octyne		0.046	0.079
173	tridecane, 6-methyl-	13287-21-3	0.59	0.10
174	c7-cyclohexane		1.1	0.1
175	tridecane, 4-methyl-	26730-12-1	0.91	0.02
176	tridecane, 2-methyl-	1560-96-9	1.3	0.04
177	undecane, 3,8-dimethyl	17301-30-3	0.021	0.037
178	c14-alkene and others		0.068	0.118
179	dodecane, 3-methyl-	17312-57-1	0.63	0.59
180	undecane, 2,8-dimethyl	17301-25-6	0.021	0.037
181	mixture		0.071	0.122
182	tridecane, 3-methyl		0.24	0.41
183	dodecane, 2,6,11-trimethyl-	31295-56-4	3.3	0.3
184	mixture		0.041	0.070
185	decane, 2-methyl	6975-98-0	0.043	0.074
186	tetradecane	629-59-4	4.1	0.2
187	pentadecane	629-62-9	1.2	0.1
188	dodecane, 2,7,10-trimethyl-	74645-98-0	0.48	0.02
189	c14-alkene and others		0.40	0.01
190	c15-alkane		0.22	0.20
191	dodecane, 2,6,11-trimethyl-	31295-56-4	0.34	0.30

192	alkane		0.10	0.17
193	pentadecane	629-62-9	0.33	0.57
194	1-pentadecene	13360-61-7	0.11	0.19
195	tridecane, 3-ethyl-	13286-73-2	0.35	0.61
196	1-octanol, 2-butyl	3913-02-8	0.11	0.18
197	tridecane, 5-propyl-	55045-11-9	1.2	1.4
198	dodecane, 3-methyl-	17312-57-1	0.15	0.26
199	tetradecane	629-59-4	0.11	0.19
200	nonane, 5-butyl-	17312-63-9	0.11	0.19
201	dodecane, 2-methyl-8-propyl	55045-07-3	1.7	1.5
202	alkane		0.14	0.24
203	c16-alkane		0.11	0.18
204	hexadecane, 3-methyl	6418-43-5	0.15	0.25
205	undecane, 5,7-dimethyl	17312-83-3	0.11	0.19
206	7-hexadecene, (Z)-	35507-09-6	0.21	0.01
207	1h-indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	54832-83-6	0.20	0.01
208	pentadecane	629-62-9	2.5	0.2
209	1h-1,2,4-triazole, 1-ethyl-	16778-70-4	0.13	0.09
210	cyclohexane, 1-(cyclohexylmethyl)-2-methyl-, cis-	54824-04-3	0.037	0.064
211	heptadecane, 2,6,10,14-tetramethyl-	18344-37-1	0.015	0.026
212	eicosane	112-95-8	0.11	0.19
213	dodecane, 2-methyl-8-propyl-	55045-07-3	0.14	0.12
214	tetradecane, 2,6,10-trimethyl	14905-56-7	0.14	0.11
215	pentadecane, 8-hexyl		0.024	0.041
216	mixture		0.087	0.112
217	hexadecane, 2-methyl-	1560-92-5	0.044	0.039
218	alkane		0.029	0.050
219	dodecane, 5,8-diethyl	24251-86-3	0.025	0.044

220	hexadecane	544-76-3	0.48	0.05
221	pentadecane, 2,6,10-trimethyl-(non-pristan)		0.063	0.055
222	ester of alkenoic acid		0.017	0.029
223	1-hexadecene	629-73-2	0.017	0.029
224	undecane, 3,6-dimethyl	17301-28-9	0.034	0.058
225	hexadecanoic acid	57-10-3	0.020	0.035
226	alkene and others		0.018	0.032
227	tetradecanoic acid	544-63-8	0.27	0.23
228	1-hexandecanol, acetate	629-70-9	0.018	0.031
229	benzenamine, N-phenyl	122-39-4	0.015	0.026
230	pentadecane	629-62-9	0.019	0.033
231	pentadecane, 2,6,10,14-tetramethyl	1921-70-6	0.019	0.033
232	tetradecanoic acid	544-63-8	0.11	0.19
233	benzenesulfonamide, n-butyl-	3622-84-2	0.38	0.04
234	9-octadecenoic acid (Z)-	112-80-1	0.030	0.026
235	9-octadecenoic acid (Z)-	112-80-1	0.016	0.028
236	14-pentadecenoic acid	17351-34-7	0.014	0.024
237	tetradecanoic acid	544-63-8	0.23	0.08
238	9-hexadecenoic acid	2091-29-4	0.52	0.14
239	hexadecanoic acid	57-10-3	1.1	0.3
240	eicosane	112-95-8	0.028	0.049
241	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.077	0.022
242	cyclohexadecane	295-65-8	0.024	0.041
243	1-hexadecanol	36653-82-4	0.039	0.067
Sum of tentatively identified compounds:			93.9	

1. CAS = Chemical Abstract Service.

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