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7. Abstract Tank 241-BY-110 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-110 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-110 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank BY-110 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-110 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-110 using the vapor sampling system (VSS) on November 11, 1994 by WHC Sampling and Mobile Laboratories, (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-BY-110 Tank Characterization Plan* (Carpenter 1994). The tank headspace temperature was determined to be 27 °C. Air from the tank BY-110 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 12B, and transferred via heated tubing to the VSS sampling manifold.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 (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^{TM,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 and SUMMATM canisters were prepared and analyzed by PNL. Clauss et al. (1995a) describe sample preparation and analyses.

¹ SUMMA is a trademark of Moleetrics, Inc., Cleveland, Ohio.

The relative standard deviations of the results, given in the last column in Table X-2, are typical for the analytical methods used. Relative standard deviations range from 2 % for water vapor, to 23 % 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, 401 ppmv, is about 16 times the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995). Ammonia is thought to be a product of chemical and radiolytic waste degradation processes. It has been observed in virtually all of the waste tanks sampled to date, at concentrations ranging from about 3 ppmv in C-108 (Lucke et al. 1995a), to 1040 ppmv in tank BY-108 (McVeety et al. 1995a).

Hydrogen and nitrous oxide are commonly detected gases in the waste tanks. Like ammonia, these are thought to be products of chemical reactions and radiolysis of the waste, and they have been found in most waste tanks headspaces sampled to date. Hydrogen was not detected in the tank BY-110 samples, being determined to be below the limit of detection of the analytical method, 160 ppmv. In general, hydrogen is of concern as a fuel. The 160 ppmv detection limit corresponds to about 0.4 % of the lower flammability limit (LFL) for hydrogen in air. The nitrous oxide concentration in tank BY-110, 103 ppmv, is about 4 times the NIOSH 8-hr REL of 25 ppmv (NIOSH 1995).

For comparison, the measured concentrations of ammonia, hydrogen, and nitrous oxide for the Ferrocyanide Watchlist tanks in 241-BY farm are given in Table X-3. Among these tanks, tank BY-110 has a moderately high level of both ammonia and nitrous oxide. There is a strong correlation between increased waste tank headspace organic vapor concentrations (the last column in Table X-3) and increased ammonia vapor concentrations, though this correlation is not linear.

X.2.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 229 ppmv, is significantly less than 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 229 ppmv carbon dioxide concentration measured in tank BY-110 is typical of other tanks sampled to date.

Carbon monoxide in the tank BY-110 headspace, measured to be < 76 ppmv, is not well characterized. The method quantitation limit, 76 ppmv, is above the highest waste tank carbon monoxide concentration measured to date (26.7 ppmv in tank C-103, Huckaby and Story 1994). Because elevated carbon monoxide concentrations are thought to be due to the decomposition of organic waste in the tanks, and tank BY-110 does not have a high organic vapor concentration, it is unlikely that the carbon monoxide concentration in the headspace is at or above the 35 ppmv, 8-hr NIOSH workplace REL (NIOSH 1995).

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

Nitric oxide and nitrogen dioxide concentrations in the tank BY-110 headspace were determined to be ≤ 0.09 ppmv and ≤ 0.05 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-110. Nitric oxide is commonly found at trace concentrations, presumably 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 was measured by gravimetric analysis of 5 sorbent trap systems by PNL (Clauss et al. 1995a). The water vapor concentration of tank BY-110 was determined to be about 8.0 mg/L, at the tank headspace temperature of 27 °C and pressure of 985 mbar (739.2 torr). This corresponds to a water vapor partial pressure of 11.1 mbar (8.3 torr), to a dew point of 8.5 °C, and to a relative humidity of 31 %.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium ions produced by the waste combine 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 9 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-110 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Both laboratories used gas chromatography and mass spectrometry (MS) to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995a) and Clauss et al. (1995a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank BY-110. 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 23 of 27 target analytes selected by WHC. Four target analytes (vinylidene chloride, dichloromethane, 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-110 are an extended set of 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). Acetone was measured to be above the method's upper calibration limit. Also, 8 of the target analytes (propanenitrile, butanal, benzene, toluene, pentanenitrile, hexanenitrile, heptanenitrile, and 2-octanone) were positively identified by ORNL, but below the method's lower calibration limit in at least 2 of the TST samples.

Also given in Table X-4 are the organic compounds positively identified and quantitated in SUMMATM canister samples by PNL. Averages reported are from analyses of 3 SUMMATM canister samples. PNL performed analyses according to the EPA task order 14 (TO-14) methodology, but expanded the number of target analytes from 40 to 55 to include waste tank analytes of particular interest (EPA 1988, Clauss et al. 1995a). Of the original 40 TO-14 analytes, only trichlorofluoromethane and 1,2,4-trichlorobenzene were determined to be above the 0.002 ppmv quantitation limit of the analyses (Clauss et al. 1995a provide the complete TO-14 analyte list). Five of the 15 additional target analytes (1-propanol, acetonitrile, butanal, propanenitrile, and butanenitrile) were below the 0.005 ppmv method quantitation limit.

Twelve target analytes were common to both the ORNL and PNL analyses. Two of these, dichloromethane and vinylidene chloride, were not detected by either laboratory. Comparison of the results from the 2 laboratories indicates the following:

- 1) The methods agree well on the concentrations of n-heptane and n-decane;
- 2) the methods are in fair agreement on the concentration of acetone, with TST analysis indicating 3.8 ppmv, and SUMMATM analysis indicating 9.9 ppmv;
- 3) n-hexane was detected by both methods, but the agreement is poor, with TST analysis indicating 0.29 ppmv, and SUMMATM analysis indicating 0.017 ppmv; and
- 4) acetonitrile, propanenitrile, butanal, benzene, butanenitrile, and toluene were reported to be below SUMMATM analysis method quantitation

limits, yet each of these were measured in TST samples to be significantly above the SUMMATM method quantitation limits.

Though the discrepancies between the TST and SUMMATM sample results exceed accuracy requirements specified in *Tank 241-BY-110 Tank Characterization Plan* (Carpenter 1994), benzene is the only analyte in question that exceeds the action limit specified by *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994). Benzene, at an average 0.034 ppmv in TST samples, is above the action level for carcinogens of one-tenth of the NIOSH 8-hr REL of 0.1 ppmv (NIOSH 1995).

The most abundant analytes in Table X-4 are acetone, acetonitrile, and 2-butanone. At the reported concentrations, the Table X-4 analytes do not individually or cumulatively represent a flammability hazard. None of the analytes in Table X-4 is above NIOSH recommended work-place guidelines.

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/m³, 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 may also determine its molecular weight. 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-5 and X-6, particularly near the bottom of the tables 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. (1995a) and Clauss et al. (1995a), 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 # 5 and 7 in Table X-6), or the assignment of the same identity to different peaks (e.g., Cmpd # 22 and 41 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.

ORNL estimated the total organic vapor concentration of tank BY-110, based on quantitative and estimated MS data, to be 29 mg/m^3 . This is comparable to analyses for total nonmethane organic carbon (TNMOC) by the EPA task order 12 (TO-12) method. The TNMOC concentration of clean ambient air ranges from about 0.03 to 0.1 mg/m^3 . TNMOC measurements of other waste tanks have ranged from as high as $5,000 \text{ mg/m}^3$ in tank C-103 (Rasmussen and Einfeld 1994), to as low as 0.18 mg/m^3 in tank C-111 (Rasmussen 1994a).

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 reside 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 in tank BY-110 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.

Though there is no toxicological or flammability hazard associated with the 0.34 ppmv of trichlorofluoromethane measured in SUMMA™ canister samples from tank BY-110, its presence warrants an explanation. The origin of trichlorofluoromethane in the waste tanks has not been established, however, it has been used as a decontaminating (cleaning) solvent at the Hanford Site, and small amounts may have been placed in the waste tanks. Once there, its high density (1.47 g/mL) and low solubility in the aqueous liquid wastes would have caused it to pool at the bottom of the tank. This analyte was also tentatively identified in the TST samples.

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

Neither TST nor SUMMA™ methods detected tributyl phosphate as a headspace constituent. The relatively high concentration of 1-butanol, however, is a strong indication that tributyl phosphate does exist in tank BY-110. That tributyl phosphate was not observed in the TST samples may be due to 1) the fact that tributyl phosphate has a very low vapor pressure and is consequently

present at a very low concentration, and 2) the tendency for tributyl phosphate to adsorb on the high efficiency particulate air (HEPA) filters used during sampling to protect the samples from radiological particulate contamination.

Volatile alkanes and alkenes are more prominent in the tank BY-110 headspace than is typical of NPH-rich tanks. For example, n-butane has the highest estimated concentration of any the tentatively identified analyte in both SUMMATM samples (Table X-5) and TST samples (Table X-6). Also, the other tentatively identified analytes in SUMMATM samples with concentrations above 1 mg/m³ are propene, propane, n-pentane, and 2-methylpentane.

In the semivolatile region of Table X-6, subjectively defined here as those compounds eluting after n-decane (Cmpd # 56 through 111), there are many branched alkanes. The abundance of these, as well as the methyl-substituted decahydronaphthalenes, has also been noted in other 241-BY farm tanks.

Table X-1
 Tank BY-110 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 blank + 2 field blank
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-110 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	401	15	4
Carbon Dioxide, CO ₂	124-38-9	SUMMA™	3	229	53	23
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 76	--	--
Hydrogen, H ₂	1333-74-0	SUMMA™	3	< 160	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.09	--	--
Nitrogen Dioxide, NO ₂	10102-44-0	Sorbent Trap	6	≤ 0.05	--	--
Nitrous Oxide, N ₂ O	10024-97-2	SUMMA™	3	103	22	21
Water Vapor, H ₂ O	7732-18-5	Sorbent Trap	6	11,300 (8.0 mg/L)	250 (0.2 mg/L)	2

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

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

Tank	Ammonia (ppmv)	Hydrogen (ppmv)	Nitrous Oxide (ppmv)	TNMOC ¹ (mg/m ³)
BY-103 ²	26	< 99	16.5	5.2
BY-104 ³	248	295	201	60.8
BY-105 ⁴	43	48	50	12.7
BY-106 ⁵	74	46	71	9.9
BY-107 ⁶	972	267	621	173
BY-108 ⁷	1040	399	641	594
BY-110 ⁸	401	< 160	103	29
BY-111 ⁹	59.2	< 160	< 67	9.6
BY-112 ¹⁰	63	< 94	40	5.8

1. TNMOC = total nonmethane organic compounds.
2. Ammonia, hydrogen, and nitrous oxide results are from McVeety et al. 1995b; TNMOC results are from Rasmussen 1994b.
3. Ammonia result is from Clauss et al. 1994; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994c.
4. Ammonia result is from Pool et al. 1995; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994d.
5. Ammonia result is from Lucke et al. 1995b; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994e.
6. Ammonia, hydrogen, and nitrous oxide results are from Clauss et al. 1995b; TNMOC result is from Rasmussen 1994f.
7. Ammonia, hydrogen, and nitrous oxide results are from McVeety et al. 1995a; TNMOC result is from Rasmussen 1994f.
8. Ammonia, hydrogen, and nitrous oxide results are from Clauss et al. 1995a; TNMOC is estimated from mass spectra data by Jenkins et al. 1995a.
9. Ammonia, hydrogen, and nitrous oxide results are from Lucke et al. 1995c; TNMOC results are from Rasmussen 1994b.

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10. Ammonia, hydrogen, and nitrous oxide results are from Clauss et al. 1995c; TNMOC is estimated from mass spectral data by Jenkins et al. 1995b.

Table X-4
Tank BY-110 Organic Target Compound Average Concentrations

Compound	CAS ¹ Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Trichlorofluoromethane	75-69-4	SUMMA ^{TM,3}	0.34	0.06	18
Ethanenitrile (acetonitrile)	75-05-8	TST ⁴ SUMMA TM	0.81 < 0.005	0.04 --	5 --
Propanone (acetone) ⁵	67-64-1	TST SUMMA TM	3.8 9.9	0.3 2.5	8 25
Propanenitrile ⁵	107-12-0	TST SUMMA TM	0.025 < 0.005	0.001 --	4 --
Butanal ⁵	123-72-8	TST SUMMA TM	0.036 < 0.005	0.007 --	19
2-Butanone	78-93-3	SUMMA TM	0.48	0.01	3
n-Hexane	110-54-3	TST SUMMA TM	0.29 0.017	0.05 0.017	18 96
Benzene ⁵	71-43-2	TST SUMMA TM	0.034 < 0.005	0.01 --	7 --
1-Butanol	71-36-3	TST	0.30	0.02	8
Butanenitrile	109-74-0	TST SUMMA TM	0.028 < 0.005	0.008 --	28 --
2-Pentanone	107-87-9	TST	0.14	0.03	20
4-Methyl-2-pentanone	108-10-1	SUMMA TM	0.0097	0.0006	7
Cyclohexane	110-82-7	SUMMA TM	0.021	0.003	13
n-Heptane	142-82-5	TST SUMMA TM	0.15 0.11	0.03 0.003	20 2
Tetrahydrofuran	109-99-9	SUMMA TM	0.15	0.002	1
Toluene ⁵	108-88-3	TST SUMMA TM	0.029 < 0.005	0.006 --	20 --
Cyclohexanone ⁶	108-94-1	SUMMA TM	0.057	--	--
1,2,4-Trichlorobenzene	120-82-1	SUMMA TM	0.0159	0.0002	1
Pentanenitrile ⁵	110-59-8	TST	0.0068	0.0011	16
2-Hexanone	591-78-6	TST	0.063	0.012	19
n-Octane	111-65-9	TST	0.061	0.008	14

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Compound	CAS ¹ Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD ² (%)
Pyridine	110-86-1	SUMMA TM	0.043	0.002	5
Hexanenitrile ⁵	628-73-9	TST	0.0058	0.0009	16
2-Heptanone	110-43-0	TST	0.056	0.008	14
n-Nonane	111-84-2	TST	0.030	0.005	15
Heptanenitrile ⁵	629-08-3	TST	0.0057	0.0013	23
2-Octanone ⁵	111-13-7	TST	0.010	0.001	10
n-Decane	124-18-5	TST	0.024	0.005	21
		SUMMA TM	0.032	0.003	9
n-Undecane	1120-21-4	TST	0.042	0.008	19
n-Dodecane	112-70-3	TST	0.079	0.012	15
n-Tridecane	629-50-5	TST	0.13	0.004	3

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. SUMMATM canister results based on analyses of 3 samples.
4. TST results are based on analyses of 3 samples.
5. Two or more of the sample results fell outside the calibration range.
6. Detected in only 1 sample.

Table X-5
Tank BY-108 Tentatively Identified Organic Compounds Reported by PNL

Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Propene	115-07-1	1.70	0.58
2	Propane	74-98-6	1.12	0.44
3	Cyclopropane	75-19-4	0.26	0.08
4	Isobutane	75-28-5	0.54	0.17
5	1-Butene	106-98-9	0.95	0.29
6	Butane	106-97-8	1.75	0.57
7	2-Methyl-1-Propene	115-11-7	0.26	0.08
8	Ethanol	64-17-5	0.19	0.06
9	2-Methyl-1-Butene	563-46-2	0.11	0.05
10	Isopropyl Alcohol ²	67-63-0	0.17	--
11	1-Pentene	109-67-1	0.59	0.33
12	Pentane	109-66-0	1.57	0.66
13	2-methyl-2-Propanol	75-65-0	0.10	0.03
14	4-Methyl-1-Pentene	691-37-2	0.16	0.04
15	2-Methylpentane	107-83-5	1.19	0.30
16	Butanol	123-72-8	0.13	0.04
17	3-Methylpentane	96-14-0	0.24	0.06
18	1-Hexene	592-41-6	0.20	0.05
19	Methylcyclopentane	96-37-7	0.15	0.04
20	Unknown Ketone		0.14	0.01
21	1-Butanol	71-36-3	0.59	0.04
22	2-Pentanone	107-87-9	0.81	0.06
23	Unknown C7 Alkane		0.48	0.01
24	1-Heptene	592-76-7	0.13	0.00
25	Unknown Alcohol ²		0.08	--
26	Unknown		0.07	0.00
27	Unknown C8 Alkane		0.29	0.00

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Cmpd #	Compound	CAS ¹ Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
28	2-Hexanone	591-78-6	0.29	0.01
29	Octane	111-65-9	0.27	0.00
30	Unknown C9 Alkane		0.10	0.00
31	Unknown C9 Alkene/Cycloalkane		0.06	0.00
32	3-Heptanone	106-35-4	0.42	0.01
33	2-Heptanone	110-43-0	0.23	0.00
34	Nonane	111-84-2	0.20	0.00
35	Unknown Ketone		0.24	0.01
36	2-Octanone	111-13-7	0.07	0.01
37	Unknown C11 Alkane		0.13	0.01
38	Unknown C10 Alkene/Cycloalkane		0.09	0.02
39	Undecane	1120-21-4	0.37	0.03
40	Unknown C11 Alkene/Cycloalkane ²		0.07	--
41	Unknown C12 Alkane ²		0.07	--
42	Dodecane	112-40-3	0.54	0.04
43	Undecane, 2,6-dimethyl-	17301-23-4	0.27	0.02
44	Unknown C13 Alkene/Cycloalkane		0.15	0.02
45	Unknown C14 Alkane		0.30	0.02
46	Tridecane	629-50-5	0.48	0.04
47	Unknown C14 Alkane		0.07	0.00
48	Unknown C13 Alkene/Cycloalkane		0.07	0.00
49	Unknown C15 Alkane		0.21	0.02
50	Tetradecane	629-59-4	0.25	0.02
Sum of tentatively identified compounds:			18.92	

1. CAS = Chemical Abstract Service.

2. Detected in only 1 sample.

Table X-6
Tank BY-110 Tentatively Identified Organic Compounds Reported by ORNL

Cmpd #	Compound	CAS Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
1	Isobutane	75-28-5	0.24	0.09
2	1-Propene, 2-methyl-	115-11-7	0.44	0.05
3	Butane	106-97-8	1.4	0.4
4	1-Propene, 2-methyl-	115-11-7	0.11	0.03
5	1-Butene	106-98-9	0.053	0.054
6	2-Butene	107-01-7	0.042	0.072
7	1-Butene	106-98-9	0.015	0.026
8	Cyclopropane, 1,2-dimethyl-, trans	2402-06-4	0.032	0.028
9	1-Butene, 2-methyl	563-46-2	0.020	0.034
10	Butane, 2-methyl-	78-78-4	0.61	0.003
11	Trichloromonofluoromethane	75-69-4	0.13	0.006
12	1-Pentene	109-67-1	0.22	0.009
13	1,3-Pentadiene, (Z)	1574-41-0	0.084	0.015
14	Isopropyl Alcohol	67-63-0	0.17	0.09
15	1-Pentene	109-67-1	0.042	0.008
16	1-Hexene	592-41-6	0.070	0.012
17	Pentane, 2-methyl-	107-83-5	0.53	0.05
18	1-Propanol	71-23-8	0.18	0.04
19	Pentane, 3-methyl-	96-14-0	0.095	0.009
20	1-Hexene	592-41-6	0.10	0.002
21	2-Butanone	78-93-3	0.22	0.10
22	1-Hexanol	111-27-3	0.029	0.050
23	Cyclohexane	110-82-7	0.019	0.033
24	Furan, tetrahydro-	109-99-9	0.19	0.13
25	Hexane, 2-methyl-	591-76-4	0.10	0.01
26	Hexane, 3-methyl-	589-34-4	0.31	0.03

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Cmpd #	Compound	CAS Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
27	1-Heptene	592-76-7	0.030	0.026
28	3-Pentanone	96-22-0	0.042	0.003
29	2-Butanone, 3,3-dimethyl	75-97-8	0.051	0.004
30	Cyclohexane, methyl	108-87-2	0.079	0.006
31	Methyl Isobutyl Ketone	108-10-1	0.074	0.003
32	Pentane, 2-cyclopropyl-	5458-16-2	0.010	0.017
33	Heptane, 3-methyl-	589-81-1	0.055	0.048
34	Cyclohexane, 1,3-dimethyl- cis-	638-04-0	0.022	0.038
35	1-Pentanol	71-41-0	0.033	0.057
36	3-Hexanone	589-38-8	0.037	0.004
37	Methanamine, N-(1-methylbutylidene)-	22431-09-0	0.015	0.026
38	Heptane, 2,6-dimethyl-	1072-05-5	0.040	0.005
39	Cyclohexane, 1,1,3-trimethyl-	3073-66-3	0.041	0.004
40	2-Hexanone, 4-methyl	105-42-0	0.027	0.024
41	1-Hexanol	111-27-3	0.088	0.004
42	4-Heptanone & C2 Benzene		0.085	0.005
43	3-Heptanone	106-35-4	0.41	0.02
44	2-Heptanone, 6-methyl	928-68-7	0.036	0.002
45	1H-Indene, octahydro-, cis-	4551-51-3	0.037	0.010
46	Octane, 2,6-dimethyl-	2051-30-1	0.029	0.025
47	Cyclohexane, propyl	1678-92-8	0.045	0.002
48	1,4-Pentadien-3-ol	922-65-6	0.009	0.016
49	2-Heptanone, 6-methyl-	928-68-7	0.18	0.01
50	Nonane, 4-methyl-	17301-94-9	0.038	0.002
51	Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	0.10	0.01
52	1-Heptanol	111-70-6	0.048	0.006
53	Cyclotetrasiloxane, octamethyl	556-67-2	0.011	0.019
54	Cyclohexane, 1-methyl-2-propyl	4291-79-6	0.042	0.009

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Cmpd #	Compound	CAS Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
55	Cyclohexane, 1-methyl-2-propyl		0.017	0.016
56	2-Nonenal, (E)-	18829-56-6	0.006	0.011
57	Nonane, 2,6-dimethyl-	17302-28-2	0.083	0.004
58	Limonene	138-86-3	0.006	0.011
59	Cyclohexane, butyl	1678-93-9	0.027	0.001
60	Cyclopropane, 1,2-dibutyl	41977-32-6	0.042	0.001
61	Heptane, 2,6-dimethyl-	1072-05-5	0.026	0.001
62	2-Heptanone, 6-methyl	928-68-7	0.013	0.012
63	Undecane, 3,4-dimethyl-	17312-78-6	0.020	0.001
64	Naphthalene, decahydro-, trans-	493-02-7	0.027	0.0003
65	Cyclohexane, 2,4-diethyl-1-methyl	61142-70-9	0.077	0.003
66	C5-cyclohexane		0.058	0.003
67	Undecane, 3,7-dimethyl-	17301-29-0	0.042	0.002
68	methyl-decahydronaphthalene		0.016	0.028
69	Undecane, 4,8-dimethyl	17301-33-6	0.016	0.028
70	Undecane, 4,7-dimethyl	55162-61-3	0.015	0.026
71	Decane, 2,3,8-trimethyl	62238-14-6	0.017	0.029
72	Naphthalene, decahydro-2-methyl	2958-76-1	0.035	0.031
73	Cyclohexane, pentyl-	4292-92-6	0.072	0.003
74	Naphthalene, decahydro-2-methyl	2958-76-1	0.059	0.002
75	Decane, 2,5-dimethyl-	17312-50-4	0.051	0.003
76	Decane, 3-methyl-	13151-34-3	0.032	0.003
77	Nonane, 5-(2-methylpropyl)-	62185-53-9	0.057	0.002
78	Decane, 3,8-dimethyl-	17312-55-9	0.042	0.0004
79	Naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.028	0.004
80	3-Dodecene, (E)-	7206-14-6	0.015	0.013
81	Naphthalene, decahydro-2,6-dimethyl	1618-22-0	0.031	0.010

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Cmpd #	Compound	CAS Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
82	Naphthalene, decahydro-1,5-dimethyl	66552-62-3	0.029	0.003
83	C6-cyclohexane		0.029	0.004
84	Undecane, 2,6-dimethyl	17301-23-4	0.25	0.01
85	Dodecane, 5-methyl- & others		0.036	0.004
86	Naphthalene, decahydro-1,6-dimethyl	1750-51-2	0.042	0.004
87	Cyclohexane, 2-butyl-1,1,3-trimethyl	54676-39-0	0.075	0.002
88	Cyclohexane, hexyl	4292-75-5	0.18	0.01
89	Dodecane, 4-methyl-	6117-97-1	0.042	0.004
90	Decane, 2,3,7-trimethyl-	62238-13-5	0.057	0.004
91	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.029	0.002
92	Tridecane, 7-methyl-	26730-14-3	0.30	0.02
93	Cyclohexane, 2,4-diethyl-1-methyl	61142-70-9	0.028	0.003
94	Cyclopentene, 5-hexyl-3,3-dimethyl-	61142-66-3	0.027	0.001
95	Undecane, 3,9-dimethyl-	17301-31-4	0.088	0.001
96	Tridecane, 6-methyl-	13287-21-3	0.007	0.012
97	Cyclohexane, octyl	1795-15-9	0.081	0.003
98	Tridecane, 2-methyl-	1560-96-9	0.047	0.002
99	Decane, 3,8-dimethyl-	17312-55-9	0.037	0.003
100	Dodecane, 2,6,11-trimethyl-	31295-56-4	0.33	0.02
101	Tetradecane	629-59-4	0.40	0.02
102	Tridecane, 4,8-dimethyl-	55030-62-1	0.047	0.004
103	C9-cyclohexane		0.043	0.002
104	Hexadecane	544-76-3	0.20	0.01
105	Pentadecane	629-62-9	0.16	0.01
106	Pentadecane, 2-methyl	1560-93-6	0.006	0.011

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Cmpd #	Compound	CAS Number	Average (mg/m ³)	Standard Deviation (mg/m ³)
107	Hexadecane	544-76-3	0.016	0.014
108	Tetradecanoic acid	544-63-8	0.043	0.022
109	Benzenesulfonamide, N-butyl	3622-84-2	0.17	0.02
110	1-Heptadecanol	1454-85-9	0.008	0.014
111	Hexadecanoic acid	57-10-3	0.043	0.046
Sum of tentatively identified compounds:			10.91	

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