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7. Abstract

Tank 241-BX-104 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. The drivers and objectives of waste tank headspace sampling and analysis are discussed in "Program Plan for the Resolution of Tank Vapor Issues" (Osborne and Huckaby 1994). Tank 241-BX-104 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-BX-104 Vapor Sampling and Analysis Tank Characterization Report

X.0 INTRODUCTION

Tank BX-104 headspace gas and vapor samples were collected and analyzed to help determine the potential risks of fugitive emissions to tank farm workers. 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 BX-104 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994). Results presented here represent the best available data on the headspace constituents of tank BX-104.

X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank BX-104 using the vapor sampling system (VSS) on December 30, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-BX-104 Tank Characterization Plan* (the TCP), (Carpenter 1994). The tank headspace temperature was determined to be 22.8 °C. Air from the BX-104 headspace was withdrawn from a single elevation via a 8.5-m long heated sampling probe mounted in riser 1, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 60 °C. All tank air samples were collected between 11:10 a.m. and 2:15 p.m., with no anomalies noted.

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 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^{TM,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 (Pool et al. 1995).

X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 235 ppmv, is almost 10 times the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv for ammonia (NIOSH 1995). Ammonia has been observed in virtually all of the passively ventilated waste tanks sampled to date, at concentrations ranging from about 3 ppmv in tank C-108 (Lucke et al. 1995), to 1040 ppmv in BY-108 (McVeety et al. 1995).

The concentration of hydrogen in tank BX-104 was determined to be < 94 ppmv. Hydrogen in the waste tanks is of concern as a fuel. Given that the lower flammability limit (LFL) for hydrogen in air is about 4 % by volume, 94 ppmv hydrogen concentration in tank BX-104 corresponds to about 0.24 % of its LFL. At this level, hydrogen is not a flammability concern in tank BX-104.

The nitrous oxide concentration in tank BX-104, 143 ppmv, is almost 6 times the NIOSH 8-hr REL of 25 ppmv for nitrous oxide (NIOSH 1995). Nitrous oxide, also known as laughing gas, has been detected in other passively ventilated waste tanks at concentrations as low as about 12 ppmv in tank TX-105 (Klinger 1995), and as high as about 800 ppmv in tank C-103 (Huckaby and Story 1994).

X.2.2 Carbon Monoxide and Carbon Dioxide

Carbon monoxide in the tank BX-104 headspace, characterized as < 12 ppmv, is below the NIOSH 8-hr REL of 35 ppmv for carbon monoxide. In ambient air it typically ranges from 0.05 to 0.15 ppmv. Because different analytical methods have been used to measure carbon monoxide in the waste tanks sampled to date, the information on carbon monoxide has varied from tank to tank. However, elevated waste tank headspace carbon monoxide concentrations are common, and are thought to be due to the decomposition of organic waste in the tanks. Carbon monoxide has not been measured at very high levels in any of the waste tanks, the highest level measured to date was 26.7 ppmv in tank C-103 (Huckaby and Story 1994).

The average carbon dioxide concentration in the tank BX-104 headspace, 74 ppmv, is significantly lower than it is in ambient air. Carbon dioxide is normally present in the ambient air at a concentration of 350 to 400 ppmv, and is typically lower than ambient 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. The 74 ppmv of carbon dioxide measured in tank BX-104 is typical for the waste tanks sampled to date.

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

Nitric oxide and nitrogen dioxide concentrations in the tank BX-104 headspace were determined to be 0.3 ppmv and ≤ 0.03 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank BX-104. The measurable presence of nitric oxide may be due to its formation from oxygen and nitrogen in the radiation field of the headspace. The NIOSH 8-hr REL is 25 ppmv for nitric oxide, and the 15-minute short term exposure limit (STEL) for nitrogen dioxide is 1 ppmv.

The water vapor concentration of tank BX-104 was determined to be about 5.9 mg/L, at the measured tank headspace temperature of 22.8 °C and pressure of 1006 mbar (754.6 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 8.1 mbar (6.1 torr), to a dew point of 4.0 °C, and to a relative humidity of 29 %.

Silica gel sorbent traps were used to test for tritium. 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. Radiochemical analysis of the silica gel trap indicated the total activity of the headspace to be less than 50 pCi/L (WHC 1995).

X.2.4 Discussion of Inorganic Gases and Vapors

Aside from water and carbon dioxide, the most abundant waste constituents in the tank BX-104 headspace are ammonia and nitrous oxide. These have been detected in most tank headspaces sampled to date, and along with hydrogen, are usually the dominate waste species.

The relative standard deviations of the inorganic gas and vapor results given in the last column in Table X-2 are generally good. Relative standard deviations range from about 1 % for ammonia to 36 % for carbon dioxide results. Because 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.), small relative standard deviations suggest proper control was maintained both in the field and in the laboratories.

X.3 ORGANIC VAPORS

Organic vapors in the tank BX-104 headspace were sampled using SUMMA^{TM} canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. Gas chromatography (GC) and mass spectroscopy (MS) were used by PNL and ORNL to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1995) and Pool et al. (1995).

SUMMA^{TM} sample results should be considered to be the primary organic vapor data for tank BX-104. ORNL analyses of TST samples from this and other waste tanks generally agree with, support, and augment the SUMMA^{TM} 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 Compounds

Positive identification of organic analytes using the methods employed by PNL and ORNL involves matching the GC retention times and MS data from a sample with that obtained when known compounds were analyzed. The concentration of an analyte in the sample is said to be quantitatively measured if the response of the GC/MS has been established at several known concentrations of that analyte (i.e., the GC/MS has been calibrated for that analyte), and the MS response to the analyte in the sample is between the lowest and highest responses to the known concentrations (i.e., the analyte is within the calibration range).

ORNL and PNL were assigned different lists of organic compounds, or target analytes, to positively identify and measure quantitatively. The ORNL target analyte list was derived from a review of the tank C-103 headspace constituents by a panel of toxicology experts (Mahlum et al. 1994). The PNL target analyte list included the 40 compounds in the Environmental Protection Agency (EPA) task order 14 (TO-14) method, which are primarily halocarbons and common industrial solvents (EPA 1988), plus 14 analytes selected mainly from the toxicology panel's review of tank C-103.

Table X-3 lists the organic compounds positively identified and quantitated in SUMMA^{TM} samples. SUMMA^{TM} analyses were performed according to the TO-14 methodology, except for methane analysis, which was analyzed with the inorganic gases (Pool et al. 1995). Only 3 of the 40 TO-14 target analytes and 10 of the 14 additional target analytes were measured to be above the 0.005 ppmv detection limit of the analyses. Averages reported are from analyses of 3 SUMMA^{TM} canister samples.

Jenkins et al. (1995) report the positive identification of 23 of 27 target analytes in TST samples. 1,1-Dichloroethene, dichloromethane, dibutyl butylphosphonate, and tributyl phosphate were the only TST target analytes not detected. The average concentrations of the detected target analytes, from the analysis of 3 TSTs, are given in Table X-4. Despite calibration of the instrument over about a 20-fold concentration range, 9 of the compounds listed in Table X-4 were outside of the calibration range in at least 2 of the TST samples.

Eleven target analytes were common to both TST and SUMMA^{TM} analyses. Table X-5 lists these, and their reported average concentrations in TST and SUMMA^{TM} samples. As indicated in Table X-5, the reported concentrations of ethanenitrile, propanenitrile, butanenitrile, benzene, toluene, n-hexane, and n-decane are each significantly higher in TST samples than in SUMMA^{TM} samples. However, none of these compounds, even assuming the higher concentration to be correct, are at or above their NIOSH 8-hr RELs.

The most abundant analytes in Tables X-3 and X-4 are 1-butanol, n-tridecane, acetone, and n-dodecane, each of which was measured to be above 1 ppmv. At the reported concentrations, the target analytes do not individually or collectively represent a flammability hazard.

X.3.2 Tentatively Identified Organic Compounds

In addition to the target analytes, the ORNL and PNL analytical procedures allow the tentative identification of other organic compounds. Tentative identification of analytes was performed 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. Many analytes can be tentatively identified with reasonable confidence without having to inject each into the GC/MS to determine their GC retention times or specific MS patterns.

By the nature of the sampling devices, virtually all organic vapors present in the tank headspace are collected by both TST and SUMMA^{TM} samples. Analyses of the samples are designed to recover, separate, and identify the organic vapors in the samples. TSTs are not good for collecting highly volatile compounds (i.e., molecules more volatile than propane), but are quite good for most others. In contrast, the recovery of very low volatility compounds (i.e., molecules with more than about 15 carbon atoms) and some polar compounds with moderate volatility (i.e., butanal) from SUMMA^{TM} samples has been problematic.

The list of tentatively identified compounds recovered from SUMMA^{TM} samples, with estimated concentrations, is given in Table X-6. Compounds are listed in Table X-6 in the order by which they eluted chromatographically, and only non-zero results are included in the reported averages. The list of tentatively identified compounds detected in TST samples, and their estimated concentrations, is given in Table X-7. Compounds are listed in Table X-7 according to the order by which the eluted chromatographically. The averages reported by ORNL in Table X-7 are all 3-sample averages, and if an analyte was not detected in a sample, its concentration in that sample was considered to be zero for averaging purposes. Estimated concentrations are in mg/m^3, based on dry air at 0 °C and 1.01 bar.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1995) and Pool et al. (1995), respectively, and should be reviewed before this data is used for decision making. The quantitative measurement 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.

Concentrations given in Tables X-6 and X-7 should be considered rough estimates. Results in Tables X-6 and X-7 are presented in terms of observed chromatographic peaks, and are not adjusted for the occurrence of split peaks or the assignment of the same identity to different peaks (e.g., Cmpd # 34 and 55 in Table X-7). In these instances, the estimated concentration of a compound appearing in more than 1 peak is simply the sum of the individual peak estimates.

On the basis of estimated concentrations, alkanes and cycloalkanes dominate the lists of tentatively identified organic compounds in tank BX-104. Ranked in order of their concentrations, these compounds account for the 12 highest compounds listed in Table X-7, and 11 of the 12 highest in Table X-6.

X.3.4 Discussion of Organic Compounds

A convenient way to consider the organic compounds listed in Tables X-3 through X-7 is to separate them into 2 categories: 1) Organic compounds added to tank BX-104 as waste that are still evaporating; and 2) organic compounds that have been generated by reactions of the original waste.

The first category encompasses all organic compounds that were placed into the tank as waste. It includes the tentatively identified alkyl-substituted decahydronaphthalenes, and semivolatile branched and straight-chain alkanes, which were used as diluents of tributyl phosphate in various plutonium extraction processes. The semivolatile straight-chain alkanes (i.e., n-undecane, n-dodecane, n-tridecane, n-tetradecane, and n-pentadecane) are often referred to in Hanford site literature as the normal paraffinic hydrocarbons (NPHs). Halogenated compounds, such as trichlorofluoromethane, were probably also placed into the waste tanks as waste. These were used as degreasing agents in various cleaning operations, and apparently were sent to the waste tanks when contaminated.

The tentatively identified cyclosiloxanes (i.e., Cmpd # 9 and 16 in Table X-7) may also be in this category. Small quantities of siloxanes may have been introduced to the waste tank through their use as process surfactants, but they may also be present in the headspace due to their use in liquid traps at the tank's breather riser.

The second category includes all organic compounds that have been generated via radiolytic and chemical reactions of the waste. The majority of compounds listed in Tables X-3 through X-7 fall into this category, including the alcohols, aldehydes, ketones, nitriles, alkenes, alkyl nitrates, and volatile alkanes, all of which have been associated with the degradation of the NPHs. While both larger and smaller molecules are generated from the waste, the most abundant of these in the headspace are the smaller, short-chain volatile compounds.

The notable absence of tributyl phosphate in the tank BX-104 samples may be due to a sampling difficulty. The abundance of the tributyl phosphate diluents and their degradation products is reason to expect tributyl phosphate to be present in the tank waste. 1-Butanol, which had the highest reported concentration of compounds in TST samples and the third highest concentration of organic compounds in SUMMA™ samples, is known to be a product of the hydrolysis of tributyl phosphate. Furthermore, informal tests by ORNL indicate that tributyl phosphate is adsorbed by the glass fiber filters used during sampling to protect the samples from radiolytic particulate contamination. Based on these considerations, the concentration of tributyl phosphate in the tank BX-104 headspace should be considered to be unknown.

The total organic vapor concentration of tank BX-104 was estimated by Jenkins et al. to be about 100 mg/m^3 from the analysis of a single TST sample by GC with flame ionization detection. A summation of concentrations of positively and tentatively identified compounds in 3 TST samples by GC/MS indicated the total organic vapor concentration to be about 85 mg/m^3. While these estimated total organic vapor concentrations are not completely equivalent to the total nonmethane organic compound (TNMOC) concentration obtained using the EPA task order 12 (TO-12) method, they are comparable. TNMOC measurements of other waste tanks have ranged from as high as 5,000 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 1994), while the TNMOC concentration of clean ambient air ranges from about 0.03 to 0.1 mg/m^3.

Jenkins et al. reported that acetone, n-dodecane, and n-tridecane were detected in the trip and field TST blanks at trace levels. The concentrations of these analytes in the TST blanks were less than 1 % of their concentrations in tank BX-104 samples. Dichloromethane was also detected in the TST blanks, but not in the tank BX-104 samples. Jenkins et al. also report that benzene and toluene were detected in the TST field blanks, at levels less than half of the tank samples.

Ambient air SUMMA™ samples collected during the tank BX-104 sampling event suggest the VSS manifold may have been contaminated with trace amounts of acetone. Specifically, analysis of an ambient air sample collect upwind of the VSS (not through the VSS manifold) indicated acetone to be present at < 0.005 ppmv, while an ambient air sample collected through the VSS (to check system cleanliness) was determined to have about 0.012 ppmv of acetone. Residual amounts of acetone, used as a cleaning solvent, may have been present in the VSS transfer tubing.

In summary, the organic vapor concentrations in tank BX-104 are relatively high. The organic vapors in tank BX-104 clearly indicate the presence of the semivolatile NPHs and their degradation products in the tank waste. Though tributyl phosphate was not detected in any of the headspace samples, there is strong evidence that it is also present in the waste.

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

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.2, 1.0, and 4.0	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 blank
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blank
	Oxidation Bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blank
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Carbon Dioxide, Carbon Monoxide, Hydrogen, Methane, Nitrous Oxide, 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 BX-104 Inorganic Gas and Vapor Concentrations

Compound	CAS[1] Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
Ammonia, NH_3	7664-41-7	Sorbent Trap	6	235	3	1
Carbon Dioxide, CO_2	124-38-9	SUMMA™	3	74	27	36
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 12	--	--
Hydrogen, H_2	1333-74-0	SUMMA™	3	< 94	--	--
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	0.3	0.02	7
Nitrogen Dioxide, NO_2	10102-44-0	Sorbent Trap	6	≤ 0.03	--	--
Nitrous Oxide, N_2O	10024-97-2	SUMMA™	3	143	7	5
Water Vapor, H_2O	7732-18-5	Sorbent Trap	6	8,100 (5.9 mg/L)	400 (0.3 mg/L)	4.7

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

Table X-3
Tank BX-104 Positively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS[1] Number	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
1	Propanenitrile (acetonitrile)[3]	75-05-8	0.052	--	--
2	Propanone (acetone)	67-64-1	1.40	0.37	26
3	Trichlorofluoromethane	75-69-4	0.14	0.042	30
4	Propanol	71-23-8	0.32	0.098	30
5	2-Butanone	78-93-3	0.22	0.010	4
6	Tetrahydrofuran	109-99-9	0.36	0.19	5
7	Butanenitrile	109-74-0	0.020	0.005	24
8	Benzene	71-43-2	0.005	0.0003	6
9	n-Heptane	142-82-5	0.067	0.001	2
10	4-Methyl-2-Pentanone	108-10-1	0.011	0.0003	3
11	Pyridine	110-86-1	0.089	0.028	31
12	Toluene	108-88-3	0.0070	0.0002	3
13	n-Decane[3]	124-18-5	0.012	--	--
14	Methane	74-82-8	< 61	--	--

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. This compound was only detected in one sample.

Table X-4
Tank BX-104 Positively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average (ppmv)	Standard Deviation (ppmv)	RSD[2] (%)
1	Ethanenitrile (acetonitrile)	75-05-8	0.34	0.02	5
2	Propanone[3] (acetone)	67-64-1	1.22	0.07	5
3	Propanenitrile	107-12-0	0.070	0.004	5
4	Butanal	123-72-8	0.36	0.13	36
5	n-Hexane	110-54-3	0.16	0.02	11
6	Benzene[3]	71-43-2	0.011	0.001	5
7	1-Butanol[3]	71-36-3	4.62	0.41	9
8	Butanenitrile	109-74-0	0.059	0.005	8
9	2-Pentanone	107-87-9	0.12	0.01	11
10	n-Heptane	142-82-5	0.067	0.011	17
11	Toluene[3]	108-88-3	0.013	0.001	7
12	Pentanenitrile[3]	110-59-8	0.023	0.002	7
13	2-Hexanone	591-78-6	0.059	0.005	8
14	n-Octane	111-65-9	0.043	0.002	5
15	Hexanenitrile[3]	628-73-9	0.020	0.002	11
16	2-Heptanone	110-43-0	0.093	0.009	10
17	n-Nonane	111-84-2	0.039	0.003	9
18	Heptanenitrile[3]	629-08-3	0.023	0.003	11
19	2-Octanone	111-13-7	0.043	0.006	13
20	n-Decane	124-18-5	0.037	0.003	7
21	n-Undecane	1120-21-4	0.26	0.01	5
22	n-Dodecane[3]	112-40-3	1.12	0.14	12
23	n-Tridecane[3]	629-50-5	2.01	0.28	14

Sum of positively identified compounds: 50.90 mg/m^3

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. Measured concentrations were outside of calibration range for 2 or more samples.

Table X-5
Tank BX-104 Comparison of Organic Compounds in TST and SUMMA™ Samples

Compound	CAS[1] Number	TST Average (ppmv)	SUMMA™ Average (ppmv)
1,1-Dichloroethene (vinylidene chloride)	75-35-4	< 0.012	< 0.005
Dichloromethane (methylene chloride)	75-09-2	< 0.027	< 0.005
Propanone (acetone)	67-64-1	1.22	1.4
Ethanenitrile (acetonitrile)	75-05-8	0.34	0.052
Propanenitrile	107-12-0	0.070	< 0.005
Butanenitrile	109-74-0	0.059	0.020
Benzene	71-43-2	0.011	0.005
Toluene	108-88-3	0.013	0.0070
n-Hexane	110-54-3	0.16	< 0.005
n-Heptane	142-82-5	0.067	0.067
n-Decane	124-18-5	0.037	0.012

1. CAS = Chemical Abstract Service.

Table X-6
Tank BX-104 Tentatively Identified Organic Compounds in SUMMA™ Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation[2] (mg/m^3)
1	Propene	115-07-1	0.35	0.17
2	Propane	74-98-6	0.32	0.03
3	Methyl nitrite	624-91-9	0.13	0.02
4	Cyclopropane	75-19-4	0.13	0.01
5	Isobutane	75-28-5	0.074	0.007
6	Methanol	67-56-1	0.40	0.04
7	1-Butene	106-98-9	0.12	0.01
8	n-Butane	106-97-8	0.41	0.04
9	2-Methylpropene	115-11-7	0.077	0.008
10	Ethanol	64-17-5	0.16	0.04
11	1-Pentene[3]	109-67-1	0.06	--
12	n-Pentane	109-66-0	0.28	0.05
13	2-Methylpentane	107-83-5	0.24	0.01
14	Butanal	123-72-8	0.42	0.08
15	2-Butanol	78-92-2	0.076	0.002
16	1-Butanol	71-36-3	5.76	0.79
17	2-Pentanone	107-87-9	0.29	0.02
18	Unknown alkylnitrile		0.22	0.06
19	1-Pentanol	71-41-0	0.078	0.012
20	2,5-Dimethylhexane	592-13-2	0.076	0.002
21	2-Hexanone	591-78-6	0.15	0.002
22	Hexanal[3]	66-25-1	0.08	--
23	Butyl nitrate	928-45-0	0.29	0.01
24	5-Methyl-2-hexanone[4]	110-12-3	0.05	< 0.01
25	1-Hexanol	111-27-3	0.091	0.007
26	3-Heptanone	106-35-4	0.36	0.02
27	2-Heptanone	10-43-0	0.19	0.01

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation[2] (mg/m^3)
28	n-Butyl ether[3]	142-96-1	0.05	--
29	3-Heptanol[3]	589-82-2	0.11	--
30	n-Nonane	111-84-2	0.12	0.01
31	Pentyl nitrate	1002-16-0	0.054	0.006
32	6-Methyl-2-heptanone	928-68-7	0.35	0.03
33	Heptanenitrile	629-08-3	0.065	0.008
34	1-Heptanol[3]	111-70-6	0.05	--
35	2-Octanone	111-13-7	0.11	0.01
36	2-Ethyl-1-hexanol	104-76-7	0.066	0.023
37	4-Methyldecane	2847-72-5	0.061	0.006
38	Unknown alkylnitrate		0.12	0.01
39	Unknown C9 ketone		0.094	0.012
40	Octanenitrile	124-12-9	0.059	0.009
41	2-Nonanone	21-55-6	0.074	0.012
42	n-Undecane	1120-21-4	1.61	0.18
43	Unknown C12 alkane		< 0.08	--
44	5-Methylundecane	1632-70-8	0.068	0.005
45	Pentylcyclohexane	4292-92-6	0.056	0.005
46	2,5-Dimethyldecane	17312-50-4	0.17	0.06
47	4-Methylundecane	2980-69-0	0.071	0.016
48	2-Methylundecane	7045-71-8	0.20	0.02
49	3-Methylundecane	1002-43-3	0.12	0.01
50	2-Decanone[3]	693-54-9	0.06	--
51	Unknown alkane		0.14	0.05
52	n-Dodecane	112-40-3	6.92	0.95
53	Decahydro-2,6-dimethyl-naphthalene	1618-22-0	0.12	0.02
54	Unknown C13 alkane		1.72	0.23
55	Unknown C13 alkane		0.20	0.02

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation[2] (mg/m^3)
56	Unknown alkyl decahydronaphthalene[4]		0.22	0.005
57	Unknown C13 alkene/ Cycloalkane		1.03	0.12
58	Unknown C13 alkane		0.35	0.03
59	Unknown C13 alkane		0.43	0.04
60	Unknown C13 alkane		0.33	0.03
61	7-Methyltridecane	26730-14-3	2.68	0.26
62	Unknown C8 cyclohexane		0.21	0.02
63	n-Tridecane	629-50-5	8.11	0.86
64	Unknown C8 cyclohexane		0.45	0.06
65	Unknown C14 alkane		0.54	0.06
66	Unknown C13 alkene/ Cycloalkane[4]		0.21	0.09
67	Unknown C7 cyclohexane[4]		0.31	0.015
68	2-Methyltridecane	1560-96-9	0.12	0.02
69	3-Methyltridecane[3]	6418-41-3	0.09	--
70	Unknown C15 alkane		0.60	0.08
71	Unknown C4 decahydronaphthalene[4]		0.19	0.005
72	n-Tetradecane	629-59-4	0.75	0.15
73	Unknown C15 alkene/ Cycloalkane[3]		0.16	--
74	Unknown C9 cyclohexane[4]		0.16	0.01
Sum of tentatively identified compounds:			39.99	

1. CAS = Chemical Abstract Service.

2. When the analyte was detected in only 2 samples, the entry is the relative difference (i.e., their difference divided by 2).

3. Detected in only one sample.

4. Detected in only two samples.

Table X-7
Tank BX-104 Tentatively Identified Organic Compounds in TST Samples

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
1	n-Butane	106-97-8	0.80	0.16
2	Ethanol and butane, 2-methyl		0.20	0.18
3	1-Propanol	71-23-8	0.48	0.02
4	2-Butanone	78-93-3	0.26	0.01
5	Nitrous acid, butyl ester	544-16-1	0.062	0.110
6	Furan, tetrahydro-	109-99-9	0.55	0.07
7	1H-Pyrazole, 3-methyl-	1453-58-3	0.23	0.05
8	1-Pentanol	71-41-0	0.062	0.110
9	Cyclotrisiloxane, hexamethyl	541-05-9	0.48	0.16
10	Nitric acid, butyl ester	928-45-0	0.17	0.01
11	1-Hexanol	111-27-3	0.17	0.03
12	3-Heptanone	106-35-4	0.54	0.05
13	Nitric acid, pentyl ester	1002-16-0	0.049	0.085
14	2-Heptanone, 6-methyl	928-68-7	0.59	0.08
15	1-Heptanol	111-70-6	0.052	0.090
16	Cyclotetrasiloxane, octamethyl	556-67-2	0.21	0.20
17	1-Hexanol, 2-ethyl-	104-76-7	0.23	0.04
18	Oxirane, 2-ethyl-3-propyl-, cis-	56052-94-9	0.16	0.02
19	2-Heptanone, 6-methyl	928-68-7	0.15	0.02
20	1-Octanol	111-87-5	0.17	0.02
21	2-Nonanone	821-55-6	0.046	0.080
22	Octane, 6-ethyl-2-methyl-	62016-19-7	0.17	0.02
23	Cyclohexane, pentyl		0.13	0.11
24	Naphthalene, decahydro-2-methyl	2958-76-1	0.037	0.064

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
25	Undecane, 6-methyl-	17302-33-9	0.36	0.05
26	Undecane, 4-methyl-	2980-69-0	0.21	0.02
27	Undecane, 2-methyl-	7045-71-8	0.41	0.05
28	Decane, 3,8-dimethyl-	17312-55-9	0.30	0.04
29	Decane, 2,4,6-trimethyl-	62108-27-4	0.20	0.02
30	Cyclohexane, 1-ethyl-4-methyl-, cis-	4926-78-7	0.57	0.06
31	Naphthalene, decahydro-2,6-dimethyl-	1618-22-0	0.039	0.068
32	4-Undecene, 6-methyl		0.24	0.01
33	Undecane, 2,6-dimethyl-	17301-23-4	2.17	0.19
34	Dodecane, 3-methyl-	17312-57-1	0.46	0.05
35	Decane, 2,3,7-trimethyl-	62238-13-5	0.16	0.02
36	Cyclododecane	294-62-2	0.16	0.01
37	Naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.039	0.068
38	4-Nonene, 5-butyl-	7367-38-6	0.085	0.074
39	Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	0.84	0.09
40	C6-Cyclohexane		1.77	0.16
41	Undecane, 2,3-dimethyl-	17312-77-5	0.78	0.11
42	Decane, 2,3,7-trimethyl-	62238-13-5	0.85	0.11
43	Cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.31	0.02
44	Octane, 2,3,7-trimethyl-	62016-34-6	3.05	0.32
45	Cyclohexane, 1,1,3,5-tetramethyl-	50876-32-9	0.15	0.27
46	2(3H)-Benzofuranone, 3a,4,5,6- tetrahydro-trimethyl	16778-26-0	0.30	0.03
47	3-Undecanone	2216-87-7	0.30	0.11
48	Tridecane, 7-methyl-	26730-14-3	0.26	0.02

Cmpd #	Compound	CAS[1] Number	Average (mg/m^3)	Standard Deviation (mg/m^3)
49	Undecane, 5,5-dimethyl-	17312-73-1	1.42	0.14
50	C3-Decahydronaphthalene		0.24	0.03
51	Cyclohexane,1,3,5-trimethyl-2-octadecyl-	55282-34-3	0.048	0.084
52	Dodecane, 2,5-dimethyl	56292-65-0	0.061	0.100
53	C7-Cyclohexane		1.07	0.07
54	Tridecane, 2-methyl-	1560-96-9	0.48	0.04
55	Dodecane, 3-methyl-	17312-57-1	0.54	0.06
56	Tetradecane, 4-methyl	25117-24-2	3.13	0.33
57	1,1'-Bicyclohexyl, 2-methyl-, cis-	50991-08-7	0.12	0.02
58	3-Dodecanone	1534-27-6	0.31	0.05
59	Tetradecane	629-59-4	3.61	0.57
60	Tridecane, 4,8-dimethyl-	55030-62-1	0.57	0.09
61	Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	54965-05-8	0.74	0.09
62	Hexadecane	544-76-3	0.55	0.10
63	6-Tridecanone	22026-12-6	0.31	0.07
64	3-Tridecanone	1534-26-5	0.17	0.06
65	Pentadecane	629-62-9	0.16	0.02
66	Benzenesulfonamide, N-butyl-	3622-84-2	0.097	0.088
Sum of tentatively identified compounds:			33.63	

[1] CAS = Chemical Abstract Service.

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