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| Project Title/Work Order | | EDT No. |
| Tank 241-C-108 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-423) | | ECN No. 623546 |

| Name | MSIN | Text With All Attach. | Text Only | Attach./ Appendix Only | EDT/ECN Only |
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Page 1 of 2

1. ECN No 623546

Proj. ECN

| 2. ECN Category (mark one) | 3. Originator's Name, Organization, MSIN, and Telephone No. | 3a. USQ Required? | 4. Date |
|---|---|---|---|
| Supplemental [] Direct Revision [X] Change ECN [] Temporary [] Standby [] Supersedure [] Cancel/Void [] | J. W. Osborne/Vapor Sampling/ S7-15/3-5379 | [] Yes [X] No | May 31, 1995 |
| | 5. Project Title/No./Work Order No. | 6. Bldg./Sys./Fac. No. | 7. Approval Designator |
| | Vapor Sampling | 200 Gen | N/A |
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| | WHC-SD-WM-ER-423 , Rev 0 | | N/A |

| 11a. Modification Work | 11b. Work Package No. | 11c. Modification Work Complete | 11d. Restored to Original Condition (Temp. or Standby ECN only) |
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| [] Yes (fill out Blk. 11b) [X] No (NA Blks. 11b, 11c, 11d) | N/A | N/A Cog. Engineer Signature & Date | N/A Cog. Engineer Signature & Date |

12. Description of Change

Addition of caveat regarding Oak Ridge National Laboratory quality assurrance assessment in the organic vapor chapter. Minor editorial changes also.

13a. Justification (mark one)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Criteria Change | [] | Design Improvement | [] | Environmental | [] | Facility Deactivation | [] |
| As-Found | [] | Facilitate Const | [] | Const. Error/Omission | [] | Design Error/Omission | [X] |

13b. Justification Details

New information regarding Oak Ridge National Laboratory analytical results pertaining to document was added.

14. Distribution (include name, MSIN, and no. of copies)

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1. ECN (use no. from pg. 1) 623546

| 15. Design Verification Required | 16. Cost Impact | | | | 17. Schedule Impact (days) | |
|---|---|---|---|---|---|---|
| | ENGINEERING | | CONSTRUCTION | | | |
| [] Yes | Additional | [] $ | Additional | [] $ | Improvement | [] |
| [X] No | Savings | [] $ | Savings | [] $ | Delay | [] |

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

| | | | | | |
|---|---|---|---|---|---|
| SDD/DD | [] | Seismic/Stress Analysis | [] | Tank Calibration Manual | [] |
| Functional Design Criteria | [] | Stress/Design Report | [] | Health Physics Procedure | [] |
| Operating Specification | [] | Interface Control Drawing | [] | Spares Multiple Unit Listing | [] |
| Criticality Specification | [] | Calibration Procedure | [] | Test Procedures/Specification | [] |
| Conceptual Design Report | [] | Installation Procedure | [] | Component Index | [] |
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| OM Manual | [] | Operational Safety Requirement | [] | ICRS Procedure | [] |
| FSAR/SAR | [] | IEFD Drawing | [] | Process Control Manual/Plan | [] |
| Safety Equipment List | [] | Cell Arrangement Drawing | [] | Process Flow Chart | [] |
| Radiation Work Permit | [] | Essential Material Specification | [] | Purchase Requisition | [] |
| Environmental Impact Statement | [] | Fac. Proc. Samp. Schedule | [] | Tickler File | [] |
| Environmental Report | [] | Inspection Plan | [] | | [] |
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| Document Number/Revision | Document Number/Revision | Document Number Revision |
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| | | |

20. Approvals

| | Signature | Date |
|---|---|---|
| **OPERATIONS AND ENGINEERING** | | |
| Cog. Eng. J. W. Osborne | | 5-31-95 |
| Cog. Mgr. T. J. Kelley | | 5-31-95 |
| QA | | |
| Safety | | |
| Environ. | | |
| Other | | |

| | Signature | Date |
|---|---|---|
| **ARCHITECT-ENGINEER** | | |
| PE | | |
| QA | | |
| Safety | | |
| Design | | |
| Environ. | | |
| Other | | |

**DEPARTMENT OF ENERGY**

Signature or a Control Number that tracks the Approval Signature

**ADDITIONAL**

# RELEASE AUTHORIZATION

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|---|---|
| **Document Number:** | WHC-SD-WM-ER-423, REV 1 |
| **Document Title:** | Tank 241-C-108 Vapor Sampling and Analysis Tank Characterization Report |
| **Release Date:** | 5/31/95 |

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

**APPROVED FOR PUBLIC RELEASE**

**WHC Information Release Administration Specialist:**

Kara M. Broz — May 31, 1995

# SUPPORTING DOCUMENT

1. Total Pages 18

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|---|---|---|
| Tank 241-C-108 Vapor Sampling and Analysis Tank Characterization Report | WHC-SD-WM-ER-423 | 1 |

| 5. Key Words | 6. Author |
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| 241-C-108, Headspace vapor samples, organic analytes, VSS, SUMMA™, inorganic gases and vapors | Name: J. L. Huckaby<br>Signature<br>Organization/Charge Code<br>75600/N4AB1 |

7. Abstract

Tank 241-C-108 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-C-108 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).





8. RELEASE STAMP

| RECORD OF REVISION | (1) Document Number WHC-SD-WM-ER-423 | Page 1 |
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(2) Title

Tank 241-C-108 Vapor Sampling and Analysis Tank Characterization Report

CHANGE CONTROL RECORD

| (3) Revision | (4) Description of Change - Replace, Add, and Delete Pages | Authorized for Release | |
|---|---|---|---|
| | EDT-159095 | (5) Cog. Engr. | (6) Cog. Mgr. Date |
| 1 RS | (7) Made editorial changes and added information in organic vapor chapter. | J.W. Osborne | T.J. Kelley 5/31-95 |
| | ECN-623546 | | |

# Tank 241-C-108 Vapor Sampling and Analysis Tank Characterization Report

## X.0 INTRODUCTION

Tank C-108 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 C-108 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 C-108 using the vapor sampling system (VSS) on August 5, 1994 by WHC Sampling and Mobile Laboratories (WHC 1995). Sample collection and analysis were performed as directed by the sample and analysis plan (WHC 1995, Appendix A). The tank headspace temperature was determined to be 25 °C. Air from the tank C-108 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 4, 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), Pacific Northwest Laboratories (PNL), and Oregon Graduate Institute of Science and Technology (OGIST) through a contract with Sandia National Laboratories. The 39 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 18 trip blanks provided by the laboratories.

A general description of vapor sampling and sample analysis methods is given by Huckaby (1995). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC 1995 and references therein.

## X.2 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA™,[1] canister tank air samples for selected inorganic gases and vapors are given in Table X-2 in parts per million by volume (ppmv). Inorganic analyte sorbent traps were prepared and analyzed by PNL. SUMMA™ canisters were analyzed for inorganic analytes by

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

OGIST. Reports by PNL (Lucke et al. 1995) and SNL/OGIST (Rasmussen 1994) describe sample preparation and analyses.

The small relative standard deviations of the results, given in the last column in Table X-2, indicate the precision of reported results is good. Relative standard deviations range from 0.3 % for nitrous oxide results, to 30 % for carbon monoxide results. The larger relative standard deviation of the carbon monoxide results is due to the fact that it is near the analytical method's limit of quantitation. The precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), and the small relative standard deviations suggest a high degree of control was maintained both in the field and in the laboratories.

### X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 2.7 ppmv, is lower than the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995). Ammonia concentrations have typically been observed to be higher than this level in the waste tank headspaces. The relatively low ammonia concentration in tank C-108 may be related to the fact that only a small quantity of relatively cool waste is stored in tank C-108.

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 15.3 ppmv of hydrogen in tank C-108, however, represents only about 0.04 % 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 C-108, 344 ppmv, is almost 14 times the NIOSH 8-hr REL of 25 ppmv (NIOSH 1995).

### X.2.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 16.3 ppmv, is markedly lower than normal ambient air concentrations of about 400 ppmv. Little data on waste tank headspace carbon dioxide concentrations is available, but lower than ambient concentrations are expected. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. It is reasonable to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial liquid, and condensate) in the tank. For comparison, the carbon dioxide concentrations of the cascaded tanks BY-104, BY-105, and BY-106 are 10.5 ppmv, 94 ppmv, and 47.6 ppmv, respectively (Rasmussen 1994b, 1994c, 1994d).

Carbon monoxide in the tank C-108 headspace, at about 0.10 ppmv, is about the same as in ambient air, where it typically ranges from 0.05 to 0.15 ppmv.

Elevated waste tank headspace carbon monoxide concentrations are common (e.g., carbon monoxide concentration in tank C-103 was 26.7 ppmv, Huckaby and Story 1994), and are thought to be due to the decomposition of organic waste in the tanks. The relatively low carbon monoxide in tank C-108 may be due to the fact that the tank has a relatively small, cool waste inventory.

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

Nitric oxide and nitrogen dioxide concentrations in the tank C-108 headspace were determined to be 0.24 ppmv and ≤ 0.04 ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH sludge in tank C-108. 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 C-108 was determined to be about 17.5 mg/L, at the tank headspace temperature of 25 °C and pressure of 990 mbar (743 torr), (WHC 1995). This corresponds to water vapor partial pressure of 24.1 mbar (18.1 torr), to a dew point of 20.5 °C, and to a relative humidity of 76 %.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium produced by the waste combines with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Analysis of the silica gel, which would have trapped approximately 20 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 C-108 headspace were sampled using SUMMA™ canisters, which were analyzed at PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. None of the positively or tentatively identified organic analytes were at or above levels of concern. Both laboratories used gas chromatography and mass spectrometry to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994) and Lucke et al. (1995). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method was also performed by OGIST (EPA 1988, Rasmussen 1994a).

SUMMA™ sample results should be considered to be the primary organic vapor data for tank C-108. ORNL analyses of TST samples from this and other waste tanks generally agree with, support, and augment the SUMMA™ sample results. However, because certain WHC quality assurance requirements were not satisfied

by ORNL, the quality assurance assessment of ORNL by Hendrickson (1995) should be reviewed before results unique to the TST samples are used for decision making.

### X.3.1 Positively Identified Organic Analytes

ORNL positively identified and quantitated 17 of 27 analytes selected by WHC, (10 analytes were below detection limits). These analytes, and their average concentrations from the analysis of 5 TSTs, are given in Table X-3. The 27 TST target analytes for tank C-108 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). Of the 17 analytes positively identified by ORNL, only acetone was within the calibration range of the method. The other 16 positively identified analytes were at concentrations lower than the calibration range, and their concentrations should be considered to be estimated.

Also given in Table X-3 are the organic compounds positively identified and quantitated in SUMMA™ canister samples by PNL and OGIST. PNL performed analyses according to the EPA TO-14 methodology (EPA 1988, Lucke et al. 1995). Only 2 of the 40 TO-14 analytes were observed to be above the 0.002 ppmv quantitation limit of the analyses (Lucke et al. 1995 provide the complete TO-14 analyte list), and 1 of these analytes, 1,1,2-trichloro-1,2,2-trifluoroethane, is thought to be a contaminant of analysis. The results for methane are those of OGIST (Rasmussen 1994a). Averages reported are from analyses of 3 SUMMA™ canister samples except where noted.

Three target analytes were common to both the ORNL and PNL analyses: dichloromethane, benzene, and toluene. Neither ORNL nor PNL detected dichloromethane. ORNL detected trace amounts of benzene and toluene, but these were both below the limit of detection of PNL (0.002 ppbv).

The 2 most abundant analytes in Table X-3 are methane and acetone. At 0.67 ppmv, the methane concentration in tank C-108 is at about the level as ambient air. Elevated methane concentrations have been observed in other waste tank headspaces, and methane is probably formed during the chemical and radiolytic degradation of organic wastes. Acetone, at 0.018 ppmv, presents virtually no flammable or toxicological risks.

### X.3.2 Tentatively Identified Organic Analytes

In addition to targeted analytes, both ORNL and PNL analytical procedures allow the tentative identification of other organic vapors. By the nature of the samples and their analysis, virtually all 3 to 15 carbon organic compounds present in the tank headspace above analytical detection limits are observable. The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table X-4, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table X-5. 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-5, particularly near the bottoms of the table where the analytes have higher molecular weights, illustrate this.

The PNL and ORNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and Lucke et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-4 and X-5 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 30 and 32 in Table X-5). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

Concentrations given in Tables X-4 and X-5 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

### X.3.3 Total Nonmethane Organic Compounds

OGIST measured the total nonmethane organic compound (TNMOC) concentration in 3 SUMMA™ canister samples using the EPA TO-12 method (Rasmussen 1994a). The sample mean was 0.35 $mg/m^3$, with a standard deviation of 0.02 $mg/m^3$. Though data on other tanks is very limited, this value is very low compared to most other waste tanks sampled to date. For comparison, the TNMOC concentration in clean ambient air may range from 0.030 to 0.100 $mg/m^3$.

### X.3.4 Discussion of Organic Analytes

In general, the organic analytes observed in the waste tank headspaces are indicative of the types of organic waste that have been stored in each tank. Examination of the data provides clues to both the current organic constituents and the chemical reactions that they undergo.

Some of the compounds listed in Tables X-3, X-4, and X-5 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are tributyl phosphate, which was used as an extractant in several Hanford processes; dibutyl butylphosphonate, which was a contaminant of tributyl phosphate; and the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-undecane, n-dodecane, n-tridecane, and n-pentadecane) that were used as a diluent for tributyl phosphate.

Notably absent from the tank C-108 headspace are the semivolatile cyclic alkanes (e.g., methylated decahydronaphthalenes, cyclopentanes, and cyclohexanes) that have been observed in the 241-BY tank farm. This suggests that, like tank C-103, the semivolatile organic waste in tank C-108 may be from the Plutonium Uranium Extraction (PUREX) process, which in the late 1960's used a relatively pure form of semivolatile NPHs as a process diluent.

Most of the compounds in Tables X-3, X-4, and X-5 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.

There is an apparent correlation between acetone and 1-butanol in the waste tank headspaces, and tanks which have higher than average organic vapor concentrations tend to have both high acetone and high 1-butanol concentrations. In tank C-108, however, the 1-butanol concentration is only about 3 % of the acetone concentration.

Examination of the compounds listed in Tables X-3, X-4 and X-5 suggests many of the volatile species (presumed to be degradation products of the NPHs) have functional groups on the molecule's first or second carbon atom. For example, most alkenes listed have their double bond between the first and second carbon atoms, and ketones generally have the double bonded oxygen atom on the second carbon atom.

Though their concentrations are not significant, many alcohols and acids were tentatively identified by ORNL (Table X-5). These have generally not been observed to be as numerous in other NPH-rich tank headspaces, which tend to be dominated by aldehydes, ketones, and alkenes.

**Table X-1**
**Tank C-108 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 | 2.0 and 4.0 | Organic vapors | 8 tank air samples + 6 trip blanks |
| Oregon Graduate Institute of Science and Technology | SUMMA™ canister | 6.0 | Hydrogen, Nitrous Oxide, Carbon Dioxide, Carbon Monoxide | 3 tank air samples |
| Pacific Northwest Laboratories | Acidified Carbon Sorbent Trap | 3.0 | Ammonia | 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 C-108 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[3] | 6 | 2.7 | 0.3 | 11 |
| Carbon Dioxide, $CO_2$ | 124-38-9 | SUMMA™,[4] | 3 | 16.3 | 1.5 | 9 |
| Carbon Monoxide, CO | 630-08-0 | SUMMA™ | 3 | 0.10 | 0.03 | 30 |
| Hydrogen, $H_2$ | 1333-74-0 | SUMMA™ | 3 | 15.3 | 1.2 | 8 |
| Nitric Oxide, NO | 10102-43-9 | Sorbent Trap | 6 | 0.24 | 0.01 | 4 |
| Nitrogen Dioxide, $NO_2$ | 10102-44-0 | Sorbent Trap | 6 | ≤ 0.04 | -- | -- |
| Nitrous Oxide, $N_2O$ | 10024-97-2 | SUMMA™ | 3 | 344 | 1 | 0.3 |
| Water Vapor, $H_2O$ | 7732-18-5 | Sorbent Trap | 6 | 24,300 (17.5 mg/L) | 2,100 (1.5 mg/L) | 10 |

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

3. Sorbent trap results by PNL (Lucke et al. 1994).

4. SUMMA™ canister results by OGIST (Rasmussen 1994a).

**Table X-3**
**Tank C-108 Positively Identified Organic Compound Average Concentrations**

| Compound | CAS[1] Number | Sample Type | Average (ppmv) | Standard Deviation (ppmv) | RSD[2] (%) |
|---|---|---|---|---|---|
| Methane | 74-82-8 | SUMMA™[3,4] | 0.67 | 0.01 | 0.1 |
| Trichlorofluoromethane | 75-69-4 | SUMMA™ | 0.0095 | 0.00014 | 2 |
| 1,1,2-Trichloro-1,2,2-trifluoroethane[5] | 76-13-1 | SUMMA™ | 0.0087 | 0.00060 | 7 |
| Ethanenitrile[6] (acetonitrile) | 75-05-8 | TST[7] | 0.0052 | 0.0032 | 61 |
| Propanone (acetone) | 67-64-1 | TST | 0.018 | 0.019 | 110 |
| n-Hexane[6] | 110-54-3 | TST | 0.00029 | 0.00064 | 224 |
| Benzene[6] | 71-43-2 | TST | 0.00038 | 0.00030 | 79 |
| | | SUMMA™ | <0.002 | -- | -- |
| 1-Butanol[6] | 71-36-3 | TST | 0.00049 | 0.00060 | 121 |
| n-Heptane[6] | 142-82-5 | TST | 0.00013 | 0.00030 | 224 |
| Toluene[6] | 108-88-3 | TST | 0.00024 | 0.00047 | 192 |
| | | SUMMA™ | <0.002 | -- | -- |
| 2-Hexanone[6] | 591-78-6 | TST | 0.00012 | 0.00024 | 193 |
| n-Octane[6] | 111-65-9 | TST | 0.00014 | 0.00028 | 201 |
| 2-Heptanone[6] | 110-43-0 | TST | 0.00016 | 0.00028 | 174 |
| n-Nonane[6] | 111-84-2 | TST | 0.00021 | 0.00028 | 136 |
| Octanenitrile[6] | 124-12-9 | TST | 0.000012 | 0.000026 | 224 |
| Nonanenitrile[6] | 2243-27-8 | TST | 0.000081 | 0.000077 | 95 |

| | | | | | |
|---|---|---|---|---|---|
| n-Dodecane[6] | 112-40-3 | TST | 0.00053 | 0.00058 | 110 |
| n-Tridecane[6] | 629-50-5 | TST | 0.0011 | 0.0011 | 97 |
| Dibutyl butylphosphonate[6] | 75-46-4 | TST | 0.000008 | 0.000004 | 55 |
| Tributyl phosphate[6] | 126-73-8 | TST | 0.000075 | 0.000069 | 92 |
| Sum of nonmethane positively identified compounds: | | | 0.045 | | |

1. CAS = Chemical Abstract Service.

2. RSD = relative standard deviation.

3. Methane analyses by OGIST (Rasmussen 1994a), all other SUMMA™ canister results by PNL (Lucke et al. 1994).

4. SUMMA™ canister results based on analyses of 3 samples.

5. Suspect contamination.

6. Two or more samples fell outside of calibration range.

7. TST results are based on analyses of 5 samples, except where noted.

**Table X-4**
**Tank C-108 Tentatively Identified Organic Compounds in SUMMA™ Samples**

| Cmpd # | Compound | CAS[1] Number | Average $mg/m^3$ | Standard Deviation $mg/m^3$ |
|---|---|---|---|---|
| 1 | Ethanenitrile (acetaldehyde) | 75-07-0 | 0.10 | 0.02 |
| 2 | Propanone (acetone) | 67-64-1 | 0.09 | 0.03 |
| Sum of tentatively identified compounds: | | | 0.19 | |

1. CAS = Chemical Abstract Service.

**Table X-5**
**Tan C-108 Tentatively Identified Organic Compounds in TST Samples**

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) |
|---|---|---|---|
| 1 | 1-Butene | 106-98-9 | 0.038 |
| 2 | Methane, trichlorofluoro | 75-69-4 | 0.042 |
| 3 | Acetic Acid | 64-19-7 | 0.083 |
| 4 | Acetic Acid | 64-19-7 | 0.038 |
| 5 | Propanoic acid | 79-09-4 | 0.003 |
| 6 | Hexanal | 66-25-1 | 0.010 |
| 7 | Cyclotrisiloxane, hexamethyl | 541-05-9 | 0.026 |
| 8 | Alkanone | | 0.012 |
| 9 | Heptanal | 111-71-7 | 0.009 |
| 10 | 4H-1,2,4-Triazol-3-amine, 4-ethyl | 42786-06-1 | 0.004 |
| 11 | Ethanol, 2-Butoxy | 111-76-2 | 0.001 |
| 12 | Cyclobutane, 1,1,2,3,3-pentamethyl | 57905-86-9 | 0.002 |
| 13 | Cyclotetrasiloxane, octamethyl | 556-67-2 | 0.020 |
| 14 | Benzene, (1-methylethenyl)- | 98-83-9 | 0.001 |
| 15 | Octanal | 124-13-0 | 0.016 |
| 16 | 1-Hexanol, 2-Ethyl | 104-76-7 | 0.006 |
| 17 | 1-Octanol | 111-87-5 | 0.004 |
| 18 | Ethanone, 1-phenyl | 98-86-2 | 0.001 |
| 19 | Benzenemethanol, a,a-dimethyl | 617-94-7 | 0.006 |
| 20 | Nonanal | 124-19-6 | 0.018 |
| 21 | Benzoic acid, 2-[trimethylsilyl)oxy]-trimeth | 3789-85-3 | 0.002 |
| 22 | 1-Nonanol | 143-08-8 | 0.002 |
| 23 | Decanal | 112-31-2 | 0.011 |
| 24 | Benzenamine, N-phenyl | 122-39-4 | 0.001 |
| 25 | 1,3,5,7-Tetraazatricyclo[3.3.1.13,7]decane | 100-97-0 | 0.001 |
| 26 | 2,5-Pyrrolidinedione, 1-methyl | 1121-07-9 | 0.001 |
| 27 | Undecanal | 112-44-7 | <0.001 |

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) |
|---|---|---|---|
| 28 | Decanoic acid | 334-48-5 | <0.001 |
| 29 | Alkane | | <0.001 |
| 30 | Butanoic acid, butyl ester and siloxane | 109-21-7 | <0.001 |
| 31 | Alkane | | 0.002 |
| 32 | Butanoic acid, butyl ester | 109-21-7 | <0.001 |
| 33 | n-Tetradecane | 629-59-4 | 0.002 |
| 34 | Dodecanal | 112-54-9 | <0.001 |
| 35 | Mixture | | <0.001 |
| 36 | Decane, 1,1'-oxybis | 2456-28-2 | <0.001 |
| 37 | 5,9-Undecadio-2-one, 6,10-dimethyl-,(Z) | 3879-26-3 | 0.002 |
| 38 | 2,5-Cyclohexadiene, 1,4-dione, 2,6-bis(1 | 719-22-2 | <0.001 |
| 39 | Alkanol and alkyl benzene | | 0.001 |
| 40 | C12-Alkene | | 0.003 |
| 41 | Alkene | | <0.001 |
| 42 | 2,5-Cyclohexadiene-1,4-dione, 2,6-bis | 719-22-2 | 0.002 |
| 43 | n-Hexadecane | 544-76-3 | 0.001 |
| 44 | Tetradecanoic acid | 544-63-8 | 0.002 |
| 45 | Decanoic acid | 334-48-5 | <0.001 |
| 46 | Dodecanoic acid | 143-07-7 | 0.010 |
| 47 | n-Tetradecane | 629-59-4 | <0.001 |
| 48 | Dodecane, 2-methyl-6-propyl | 55045-08-4 | 0.003 |
| 49 | Propanoic acid, 2-methyl-1(1,1-dimethyle | 74381-40-1 | 0.017 |
| 50 | Benzenamine, N-phenyl | 122-39-4 | 0.009 |
| 51 | Hexadecanamide | 629-54-9 | 0.001 |
| 52 | N-Hexyl-benzene-sulfonamide | | 0.003 |
| 53 | para-T-Butyl Benzoic acid, methyl ester | | 0.002 |
| 54 | 1,2-Benzenedicarboxylic acid, bis-(2ethyl | 117-81-7 | 0.001 |
| 55 | Octadecanoic acid | 57-11-4 | 0.001 |
| 56 | Mixture | | 0.001 |

| Cmpd # | Compound | CAS[1] Number | Average ($mg/m^3$) |
|---|---|---|---|
| 57 | 1-Hexadecanol and others | | 0.002 |
| 58 | Mixture (alkane and alkanoic acid) | | 0.002 |
| 59 | Mixture | | 0.002 |
| 60 | 9-Octadecenoic acid, (Z)- | 112-80-1 | 0.003 |
| 61 | 1,1'-Biphenyl, 2,2'-diethyl | 13049-35-9 | 0.001 |
| 62 | Tetradecanoic acid | 544-63-8 | 0.055 |
| 63 | Benzenesulfonamide, N-butyl | 3622-84-2 | 0.132 |
| 64 | Tetradecanoic acid, 12-methyl, (S) | 5746-58-7 | 0.005 |
| 65 | Cyclohexanol, 1,1'-dioxybis-and others | | <0.001 |
| 66 | Pentadecanoic acid | 1002-84-2 | 0.023 |
| 67 | C14-Alkene | | 0.016 |
| 68 | 1-Hexadecanol | 36653-82-4 | 0.012 |
| 69 | Alkanol | | 0.001 |
| 70 | n-Hexadecane | 544-76-3 | 0.001 |
| 71 | Alkane | | 0.004 |
| 72 | 9-Hexadecenoic acid | 2091-29-4 | 0.062 |
| 73 | Hexadecanoic acid | 57-10-3 | 0.120 |
| 74 | 1,2-Benzenedicarboxylic acid, butyl 2-me | 17851-53-5 | 0.004 |
| 75 | Alkanol | | <0.001 |
| 76 | 1-Hexadecanol | 36653-82-4 | 0.001 |
| 77 | 1-Hexadecanol, acetate | 629-70-9 | 0.002 |
| 78 | 1-Hexadecanol, 2-methyl | 2490-48-4 | 0.002 |
| 79 | Hexadecanoic acid | 57-10-3 | 0.002 |
| 80 | Hexadeanoic acid, 1-methylethyl ester | 142-91-6 | 0.007 |
| Sum of tentatively identified compounds: | | | 0.881 |

1. CAS = Chemical Abstract Service.

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