

A Survey of Vapors in the Headspace of Single-Shell Waste Tanks

L. M. Stock
J. L. Huckaby

July 2004



Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RL01830

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes **any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.** Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

operated by

BATTELLE

for the

UNITED STATES DEPARTMENT OF ENERGY

under Contract DE-AC06-76RL01830



This document was printed on recycled paper.

(8/00)

A Survey of Vapors in the Headspace of Single-Shell Waste Tanks

L. M. Stock
J. L. Huckaby

July 2004

Prepared for
the U.S. Department of Energy
under Contract DE-AC06-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Summary

This report summarizes data on the organic vapors in the single-shell, high-level radioactive waste tanks at the Hanford Site. The highest reported concentration of each unambiguously identified gas and vapor in the single-shell tank headspaces is provided in Tables 1 through 20. This report also indicates each tank in which the highest concentration was reported and the number of tank headspaces in which each species has been identified. Organic vapors were sorted by chemical class and arranged according to their structural similarities.

Acknowledgments

The authors would like to thank Lenna Mahoney for her careful review and helpful comments, and Rosalind Schrepf for her editorial help. This report was supported by the U.S. Department of Energy under Contract DE-AC-76RL001830 with project funding provided by CH2M HILL Hanford Group, Inc.

Contents

Summary	iii
Acknowledgments.....	v
1.0 Introduction.....	1
2.0 Description of Data	3
3.0 Procedure	5
4.0 Results.....	7
5.0 Discussion	61
6.0 References	63

Tables

1	Alkanes	8
2	Cycloalkanes.....	14
3	Alkenes	19
4	Alkynes.....	25
5	Benzene, Biphenyl, Napthalene, Fluorene and Their Derivatives.....	26
6	Halogen Containing Compounds.....	28
7	Alcohols, Phenols, and Ethers	31
8	Aldehydes	35
9	Ketones	37
10	Acids.....	42
11	Esters.....	43
12	Nitriles	46
13	Amines and Amides.....	47
14	Nitrous and Nitric Acid Esters, Nitroso and Nitro Compounds	49
15	Heterocyclic Compounds.....	51
16	Sulfur Compounds	55
17	Silicon Compounds.....	56
18	Other Organic Compounds	57
19	Inorganic Compounds.....	58
20	Total Nonmethane Hydrocarbon Measurements and Summations of GC/MS Analyses	59
21	Summary of Observations	60

1.0 Introduction

This report summarizes data on the organic vapors in the single-shell, high-level radioactive waste tanks at the Hanford Site. The report was originally issued in 2000 and has been revised with new information including recent work on the determination of the organic compounds in 17 additional SUMMATM canisters from the single-shell tanks. The vast majority of data were obtained from the Tank Characterization Database (TCD) (PNNL 2004), and analyses of the 17 additional SUMMATM canisters were obtained from the laboratory reports (Bolling 2002a, 2002b, 2003a, 2003b, 2003c, 2004). The TCD contains about 41,000 results for compounds detected by gas chromatograph/mass spectrometer (GC/MS) organic vapor analyses. This report summarizes the results for about 1,230 compounds, of which about 550 were found in only one type of sample from a single tank. Of the 1,230 compounds, 445 have maximum reported concentrations of less than 0.025 mg/m³. Each single-shell tank farm and all major waste types are represented. Descriptions of the sampling and analysis methods have been given elsewhere (Huckaby et al. 1995, Huckaby et al. 1996), and references for specific data are available in the TCD.

2.0 Description of Data

The extent to which different tank headspaces have been characterized varies greatly. The majority of tanks have been sampled only once, and generally a single laboratory analyzed the samples, but some tanks have been sampled repeatedly and multiple laboratories have conducted analyses. Two types of sampling devices, triple sorbent traps (TSTs) and SUMMA™ canisters, were employed to ensure collection and recovery of organic compounds with a broad range of volatilities and to provide a comparison of overlapping results.

Analyses to identify and quantify specific organic compounds have been performed on 104 of the 109 total tanks sampled.^(a) Samples from each of these 104 tanks were analyzed using GC/MS systems, with robust methods designed to maximize the number and types of species that could be detected. Limitations of the analytical methods, such as the inability of the methods to detect formaldehyde and certain other low molecular weight species, are discussed in the Data Dictionary of the Tank Waste Information Network System (TWINS 2004). This summary report includes GC/MS results from over 2,100 tank headspace samples.

Sampling and analysis plans specified that samples be analyzed for about 50 to 65 organic target compounds. The target compounds were to be positively identified (i.e., GC retention time and mass spectra were matched to that of a known standard) and quantitatively measured (i.e., a multi-point calibration of the GC/MS was performed with known standards). Concentrations of target compounds were generally required to be accurate to within 30%. Non-target organic compounds were tentatively identified by comparing their observed mass spectra with those in the National Institute for Standards and Technology (NIST)/Wiley mass spectral library, and applying both automatic search methods and professional judgment to identify the best match. Experience indicates this method for identification of organic compounds is fairly reliable for many compounds. Ambiguities arose because gas chromatogram retention times were not always considered in assignment of chemical names. Confidence that any given tentatively identified compound has been properly identified tends to go down as its concentration goes down and as the number of possible chemical isomers goes up. Concentrations of tentatively identified compounds were estimated by comparing their instrument response to that of chromatographically adjacent internal standards, and generally, should be considered only accurate to a factor of 2.

In addition to uncertainties in the sampling and analysis methodology, changes in the ventilation rates of the single-shell tanks directly affect the headspace concentrations of all species. If a given tank were sampled during a period when its ventilation rate was low, the measured concentrations would be higher than if the tank were sampled during a period of high ventilation rate. Ventilation rates of both the passively and actively ventilated tanks may vary by a factor of about 3 due to vent-and-balance adjustments and meteorological conditions, and the reported concentrations should be assumed to vary accordingly.

-
- (a) In 1995, it was decided that organic vapor speciation would not be conducted on certain tanks if their total organic vapor concentration was below 5 mg/m³.
- (b) Single shell tanks C-104, C-105, C-106, SX-101, SX-102, SX-103, SX-104, SX-105, SX-106, SX-107, SX-108, SX-109, SX-110, SX-111, SX-113, and SX-115 were actively ventilated during the initial headspace sampling events in the 1990s. Passive ventilation rates are discussed by Huckaby et al. 1998.

3.0 Procedure

Tank headspace gas and vapor data from the TCD and the industrial hygiene samples were compiled into a single data file. Suspect results (flagged by the analyst as suspect or associated with blank contamination or results for target analytes that were below the detection limit) were not included in the report. Similarly, the results for ambiguously identified species (e.g., species identified as “unknown,” “unknown C-12 alkanone,” etc.) were excluded. Sometimes two or more compounds elute simultaneously from the GC/MS system, and the database therefore contains entries such as “dodecane and 2'-hydroxy-5'-methoxyacetophenone.” Any compound identified only in a mixture (i.e., not reported in any tank except as part of a mixture) was excluded from this report, and the reported concentrations of all mixtures were excluded from consideration in determining the maximum concentration observed.^(a)

Results for individual organic compounds have been divided into 18 tables according to chemical classification. Individual tables are given for the alkanes; cycloalkanes; alkenes and alkadienes; alkynes; arenes; halogen compounds; alcohols, phenols, and ethers; aldehydes; ketones; acids; esters; nitriles; amines and amides; nitroso and nitro compounds; heterocycles; sulfur-containing compounds; silicon compounds; and miscellaneous organic compounds. This categorization was accomplished readily because there are very few compounds with more than one functional group. In the few cases where a compound could be included in more than one table, the compounds were included in the table of perceived greater toxicological interest (in only one table). For example, the haloalkene chloroethene was included in the halogen-containing compound table (Table 6) and not in the alkene table (Table 3).

Table 19 lists results for inorganic compounds. The tanks having the highest total organic vapor concentrations are listed in Table 20 with the reported values. Summary statistics are given in Table 21.

(a) An exception to this rule is the m-xylene, p-xylene mixture, which is included in this report.

4.0 Results

The observations for the alkanes, cycloalkanes, alkenes and alkadienes, alkynes, arenes, halogenated compounds, alcohols, phenols and ethers, aldehydes, ketones, acids, esters, amines and amides, nitriles, nitroso and nitro compounds, heterocycles, silicon compounds, sulfur compounds, and miscellaneous organic compounds appear in Tables 1 to 18. Table 19 lists the inorganic compounds.

The compounds are assembled in the tables beginning with the smallest molecular weight. The next columns show the total number different tanks in which the compound was detected, the maximum observed concentration in mg/m³, the molecular weight, the maximum observed concentration in ppbv, and the tank from which the sample having the maximum concentration was obtained. The sums of the total number of observations and the maximum concentrations appear at the bottom of each table.

Table 20, which is also derived from information in the TCD, lists the 10 tanks with the highest total concentrations of organic carbon based on three different analytical measurements. The total nonmethane hydrocarbon (TNMHC) measurement was conducted by analysis of SUMMATM canister samples using the U.S. Environmental Protection Agency (EPA) Task Order 12 (TO-12) method. Summations of the reported concentrations by GC/MS analysis of SUMMATM and TST samples are also given.

Finally, Table 21 provides a summary of the results. This table provides perspective on the total number of different compounds in different structural categories and the number of compounds observed in only one tank. The table lists the sum of the maximum concentrations of the compounds in the category in ppmv. Table 21 also lists the number of compounds reported to have concentrations in excess of 100, 500, and 1,000 ppbv for each structural group.

Table 1. Alkanes

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Methane	74-82-8	15	11	16.043	17,000	241-C-103
Ethane	74-84-0	2	0.11	30.070	89	241-TX-111
Propane	74-98-6	42	8.5	44.097	4,700	241-C-105
2-Methylpropane	75-28-5	13	1.6	58.124	656	241-BY-106
2,2-Dimethylpropane	463-82-1	7	0.16	72.151	54	241-A-101
Butane	106-97-8	53	18	58.124	7,712	241-C-103
2-Methylbutane	78-78-4	12	7.2	72.151	2,454	241-BY-108
2,2-Dimethylbutane	75-83-2	8	0.56	86.178	160	241-BY-105
2,3-Dimethylbutane	79-29-8	1	0.029	86.178	8.3	241-U-107
2,2,3-Trimethylbutane	464-06-2	1	0.092	100.206	22	241-TY-104
2,2,3,3-Tetramethylbutane	594-82-1	3	0.22	114.233	47	241-BX-111
Pentane	109-66-0	47	17	72.151	5,700	241-BY-105
2-Methylpentane	107-83-5	21	14	86.178	3,901	241-BY-108
3-Methylpentane	96-14-0	12	2.3	86.178	650	241-BY-108
3-Ethylpentane	617-78-7	2	0.89	100.206	217	241-TY-104
2,2-Dimethylpentane	590-35-2	1	0.047	100.206	11	241-TY-104
2,3-Dimethylpentane	565-59-3	18	2.9	100.206	716	241-TY-101
2,4-Dimethylpentane	108-08-7	6	0.55	100.206	134	241-U-102
3,3-Dimethylpentane	562-49-2	8	1.3	100.206	313	241-TY-101
3-Ethyl-2-methylpentane	609-26-7	1	0.022	114.233	4.7	241-BY-106
2,3,3-Trimethylpentane	560-21-4	4	1.3	114.233	278	241-TX-116
2,3,4-Trimethylpentane	565-75-3	1	0.29	114.233	62	241-TX-116
Hexane	110-54-3	72	7.9	86.178	2,237	241-BY-108
2-Methylhexane	591-76-4	18	3.4	100.206	828	241-TY-101
3-Methylhexane	589-34-4	23	5.1	100.206	1,253	241-TY-101
2,3-Dimethylhexane	584-94-1	3	1.0	114.233	216	241-BY-107
2,4-Dimethylhexane	589-43-5	8	1.6	114.233	334	241-BY-108
2,5-Dimethylhexane	592-13-2	4	0.21	114.233	45	241-AX-102
2,2,3-Trimethylhexane	16747-25-4	2	0.017	128.260	3.3	241-U-107
2,2,4-Trimethylhexane	16747-26-5	1	0.011	128.260	2.1	241-TY-104
2,2,5-Trimethylhexane	3522-94-9	3	0.060	128.260	11	241-SX-107
2,3,3-Trimethylhexane	16747-28-7	1	0.0018	128.260	0.35	241-T-107
2,3,5-Trimethylhexane	1069-53-0	6	0.27	128.260	52	241-BX-103
2,2,5,5-Tetramethylhexane	1071-81-4	1	0.024	142.287	4.1	241-U-106
3,3,4,4-Tetraethylhexane	5171-86-8	1	0.075	198.395	9.3	241-BY-107

Table 1. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Heptane	142-82-5	70	4.0	100.206	984	241-BY-108
2-Methylheptane	592-27-8	8	1.8	114.233	392	241-BY-108
3-Methylheptane	589-81-1	12	0.51	114.233	110	241-BY-108
3-Ethylheptane	15869-80-4	2	0.035	128.260	6.6	241-T-111
4-Methylheptane	589-53-7	2	1.8	114.233	392	241-C-103
2,3-Dimethylheptane	3074-71-3	6	0.26	128.260	49	241-BY-108
2,4-Dimethylheptane	2213-23-2	9	0.61	128.260	117	241-BY-101
2,5-Dimethylheptane	2216-30-0	3	0.11	128.260	21	241-TX-116
2,6-Dimethylheptane	1072-05-5	6	0.50	128.260	96	241-BY-108
3,3-Dimethylheptane	4032-86-4	1	0.017	128.260	3.3	241-C-110
3,5-Dimethylheptane	926-82-9	1	0.20	128.260	38	241-BY-108
2,2,4-Trimethylheptane	14720-74-2	4	0.66	142.287	113	241-TX-116
2,3,5-Trimethylheptane	20278-85-7	1	1.7	142.287	299	241-BY-108
2,3,6-Trimethylheptane	4032-93-3	2	1.7	142.287	299	241-BY-108
3,3,5-Trimethylheptane	7154-80-5	4	0.21	142.287	36	241-AX-104
2-Methyl-3-ethylheptane	14676-29-0	7	0.067	142.287	11	241-BY-104
2-Methyl-5-ethylheptane	13475-78-0	1	0.041	142.287	7.1	241-BY-102
5-Methyl-3-ethylheptane	52896-90-9	2	1.0	142.287	173	241-C-102
4-(1-methylethyl)heptane	52896-87-4	2	0.40	142.287	69	241-BY-108
4-Ethyl-2,2,6,6-tetramethylheptane	62108-31-0	2	0.34	184.368	45	241-AX-104
4-Propylheptane	3178-29-8	1	0.0087	142.287	1.5	241-A-102
2,2,4,6,6-Pentamethylheptane	13475-82-6	4	0.22	170.341	32	241-B-103
2,2,3,4,6,6-Hexamethylheptane	62108-32-1	1	0.013	184.368	1.7	241-TY-104
Octane	111-65-9	60	1.6	114.233	353	241-C-103
2-Methyloctane	3221-61-2	3	0.018	128.260	3.5	241-BY-106
3-Methyloctane	2216-33-3	5	0.57	128.260	108	241-BY-108
4-Methyloctane	2216-34-4	5	1.1	128.260	210	241-BX-103
3-Ethyl-2,7-dimethyloctane	62183-55-5	2	0.013	170.341	1.8	241-U-107
4-Ethylloctane	15869-86-0	2	0.064	142.287	11	241-BY-109
2,5-Dimethyloctane	15869-89-3	2	0.30	142.287	52	241-C-101
2,6-Dimethyloctane	2051-30-1	6	0.30	142.287	52	241-BY-107
3,4-Dimethyloctane	15869-92-8	1	0.0080	142.287	1.4	241-BY-105
3,5-Dimethyloctane	15869-93-9	2	0.15	142.287	25	241-BY-104
2,3,3-Trimethyloctane	62016-30-2	1	0.64	156.314	100	241-BY-107
2,3,7-Trimethyloctane	62016-34-6	4	2.8	156.314	445	241-BX-104
2,5,6-Trimethyloctane	62016-14-2	2	0.028	156.314	4.4	241-U-107

Table 1. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
2-Methyl-5-ethyloctane	62016-18-6	1	0.16	156.314	26	241-C-101
2-Methyl-6-ethyloctane	62016-19-7	5	0.27	156.314	42	241-BY-108
Nonane	111-84-2	62	1.6	128.260	297	241-C-103
2-Methylnonane	871-83-0	2	0.12	142.287	20	241-BY-107
3-Methylnonane	5911-04-6	3	0.22	142.287	38	241-BY-108
4-Methylnonane	17301-94-9	10	0.65	142.287	112	241-C-102
2,6-Dimethylnonane	17302-28-2	12	3.8	156.314	602	241-C-103
4,5-Dimethylnonane	17302-23-7	2	0.0078	156.314	1.2	241-BY-105
3,7-Dimethylnonane	17302-32-8	6	2.2	156.314	344	241-BY-108
2-Methyl-5-propylnonane	31081-17-1	1	0.0018	184.368	0.24	241-T-107
3-Methyl-5-propylnonane	31081-18-2	5	0.60	184.368	80	241-U-106
5-(2-Methylpropyl)nonane	62185-53-9	2	0.052	184.368	6.9	241-BY-110
5-Propylnonane	998-35-6	1	0.0037	170.341	0.53	241-C-104
5-Butylnonane	17312-63-9	4	0.31	184.368	41	241-BY-107
2,2,4,4,6,8,8-Heptamethylnonane	4390-04-9	1	0.012	226.449	1.3	241-S-105
Decane	124-18-5	58	16	142.287	2,835	241-C-103
2-Methyldecane	6975-98-0	16	1.9	156.314	301	241-C-102
3-Methyldecane	13151-34-3	9	1.0	156.314	158	241-C-102
4-Methyldecane	2847-72-5	14	0.92	156.314	143	241-C-204
5-Methyldecane	13151-35-4	5	0.82	156.314	128	241-C-102
5-Propyldecane	17312-62-8	3	0.026	184.368	3.4	241-T-107
2,4-Dimethyldecane	2801-84-5	1	0.0030	170.341	0.43	241-BY-106
2,5-Dimethyldecane	17312-50-4	3	2.9	170.341	421	241-C-101
2,9-Dimethyldecane	1002-17-1	2	0.0078	170.341	1.1	241-A-102
3,8-Dimethyldecane	17312-55-9	5	0.27	170.341	39	241-BX-104
2,2,3-Trimethyldecane	62338-09-4	1	0.013	184.368	1.7	241-AX-102
2,2,8-Trimethyldecane	62238-01-1	2	0.26	184.368	34	241-U-106
2,3,5-Trimethyldecane	62238-11-3	3	0.04	184.368	5.7	241-BY-109
2,3,6-Trimethyldecane	62238-12-4	6	0.65	184.368	86	241-BY-108
2,3,7-Trimethyldecane	62238-13-5	3	0.92	184.368	122	241-BX-104
2,3,8-Trimethyldecane	62238-14-6	4	0.24	184.368	32	241-BY-107
2,4,6-Trimethyldecane	62108-27-4	3	22	184.368	2,918	241-C-103
2,5,9-Trimethyldecane	62108-22-9	1	0.027	184.368	3.5	241-BY-109
2,6,6-Trimethyldecane	62237-97-2	2	0.015	184.368	1.9	241-TY-104
2,6,7-Trimethyldecane	62108-25-2	4	1.3	184.368	170	241-BY-107
2,6,8-Trimethyldecane	62108-26-3	2	0.013	184.368	1.7	241-TY-104

Table 1. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
2-Methyl-6-ethyldecane	62108-21-8	1	2.0	184.368	267	241-C-102
5-Methyl-5-ethyldecane	17312-74-2	1	0.0091	184.368	1.2	241-TX-118
2,3,5,8-Tetramethyldecane	UAK014-02	1	0.15	198.395	18	241-BY-108
Undecane	1120-21-4	61	84	156.314	13,192	241-C-103
2-Methylundecane	7045-71-8	15	26	170.341	3,684	241-C-103
3-Methylundecane	1002-43-3	14	16	170.341	2,368	241-C-103
4-Methylundecane	2980-69-0	16	12	170.341	1,711	241-C-103
5-Methylundecane	1632-70-8	14	6.3	170.341	908	241-C-103
6-Methylundecane	17302-33-9	10	3.2	170.341	461	241-C-102
3-Ethylundecane	17312-58-2	1	0.0022	184.368	0.29	241-TY-104
5-Ethylundecane	17453-94-0	5	1.2	184.368	158	241-C-102
6-Ethylundecane	17312-60-6	1	0.0027	184.368	0.36	241-BY-106
2,2-Dimethylundecane	17312-64-0	1	0.015	184.368	1.9	241-U-107
2,3-Dimethylundecane	17312-77-5	3	0.89	184.368	118	241-BY-108
2,4-Dimethylundecane	17312-80-0	9	14	184.368	1,824	241-C-103
2,5-Dimethylundecane	17301-22-3	1	0.091	184.368	12	241-C-110
2,6-Dimethylundecane	17301-23-4	23	38	184.368	4,984	241-C-103
2,7-Dimethylundecane	17301-24-5	2	0.55	184.368	73	241-BY-108
2,8-Dimethylundecane	17301-25-6	4	0.78	184.368	103	241-BY-107
2,9-Dimethylundecane	17301-26-7	2	0.22	184.368	29	241-BY-107
2,10-Dimethylundecane	17301-27-8	14	36	184.368	4,741	241-C-103
3,4-Dimethylundecane	17312-78-6	2	0.65	184.368	86	241-TY-103
3,5-Dimethylundecane	17312-81-1	1	0.0009	184.368	0.12	241-C-112
3,6-Dimethylundecane	17301-28-9	2	0.092	184.368	12	241-BY-107
3,7-Dimethylundecane	17301-29-0	8	20	184.368	2,675	241-C-103
3,8-Dimethylundecane	17301-30-3	5	3.8	184.368	511	241-C-102
3,9-Dimethylundecane	17301-31-4	2	0.17	184.368	23	241-A-106
4,4-Dimethylundecane	17312-68-4	4	0.52	184.368	69	241-TY-103
4,6-Dimethylundecane	17312-82-2	3	4.8	184.368	632	241-C-101
4,7-Dimethylundecane	17301-32-5	4	2.1	184.368	280	241-BY-108
4,8-Dimethylundecane	17301-33-6	5	0.46	184.368	61	241-C-102
5,5-Dimethylundecane	17312-73-1	1	1.3	184.368	170	241-BX-104
5,7-Dimethylundecane	17312-83-3	3	0.74	184.368	98	241-TY-103
6,6-Dimethylundecane	17312-76-4	1	0.82	184.368	108	241-BY-108
Dodecane	112-40-3	62	355	170.341	51,054	241-C-103
2-Methyldodecane	1560-97-0	3	2.7	184.368	365	241-C-102

Table 1. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
3-Methyldodecane	17312-57-1	5	1.6	184.368	219	241-C-102
4-Methyldodecane	6117-97-1	15	17	184.368	2,310	241-C-103
5-Methyldodecane	17453-93-9	3	0.52	184.368	69	241-BY-108
6-Methyldodecane	6044-71-9	4	0.72	184.368	96	241-BY-108
2,5-Dimethyldodecane	56292-65-0	9	2.3	198.395	282	241-BY-108
4,6-Dimethyldodecane	61141-72-8	9	57	198.395	7,005	241-C-103
4,9-Dimethyldodecane	3054-63-5	2	0.023	254.504	2.2	241-BY-103
2,6,10-Trimethyldodecane	3891-98-3	15	54	212.422	6,225	241-C-103
2,7,10-Trimethyldodecane	74645-98-0	6	4.9	212.422	559	241-C-102
2,6,11-Trimethyldodecane	31295-56-4	11	44	212.422	5,065	241-C-103
2-Methyl-6-propyldodecane	55045-08-4	4	0.037	226.449	4.0	241-BY-104
2-Methyl-8-propyldodecane	55045-07-3	8	2.7	226.449	287	241-BY-108
5,8-Diethyldodecane	24251-86-3	2	0.070	226.449	7.5	241-BY-107
2,2,4,9,11,11-Hexamethyldodecane	6304-50-3	1	0.015	254.504	1.4	241-S-105
Tridecane	629-50-5	68	465	184.368	61,759	241-C-103
2-Methyltridecane	1560-96-9	19	19	198.395	2,373	241-C-103
3-Methyltridecane	6418-41-3	9	11	198.395	1,356	241-C-103
4-Methyltridecane	26730-12-1	13	1.4	198.395	169	241-BY-108
5-Methyltridecane	25117-31-1	4	11	198.395	1,356	241-C-103
6-Methyltridecane	13287-21-3	14	27	198.395	3,276	241-C-103
7-Methyltridecane	26730-14-3	14	11	198.395	1,356	241-BY-108
2,5-Dimethyltridecane	56292-66-1	1	0.0078	212.422	0.90	241-BY-103
4,8-Dimethyltridecane	55030-62-1	9	2.0	212.422	232	241-BY-108
3-Ethyltridecane	13286-73-2	3	1.0	212.422	116	241-BY-107
5-Propyltridecane	55045-11-9	4	1.7	226.449	188	241-BY-107
Tetradecane	629-59-4	58	111	198.395	13,670	241-C-103
3-Methyltetradecane	18435-22-8	5	0.35	212.422	40	241-BY-108
4-Methyltetradecane	25117-24-2	4	2.8	212.422	327	241-BX-104
5-Methyltetradecane	25117-32-2	1	0.0018	212.422	0.21	241-T-107
4-Ethyltetradecane	55045-14-2	1	0.037	226.449	4.0	241-BY-104
2,5-Dimethyltetradecane	56292-69-4	1	0.0092	226.449	1.0	241-BY-103
4,11-Dimethyltetradecane	55045-12-0	3	0.0092	226.449	1.0	241-BY-105
6,9-Dimethyltetradecane	55045-13-1	1	0.0009	226.449	0.10	241-T-107
2,6,10-Trimethyltetradecane	14905-56-7	4	0.17	240.476	18	241-BY-107
Pentadecane	629-62-9	33	34	212.422	3,904	241-C-103
2-Methylpentadecane	1560-93-6	6	0.30	226.449	33	241-C-102

Table 1. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
3-Methylpentadecane	2882-96-4	1	0.059	226.449	6.3	241-C-110
2,6,10-Trimethylpentadecane	3892-00-0	5	0.086	254.504	8.3	241-BY-107
2,6,10,14-Tetramethylpentadecane	1921-70-6	5	0.052	268.531	4.8	241-BY-107
8-Hexylpentadecane	13475-75-7	2	0.066	296.585	5.4	241-BY-107
Hexadecane	544-76-3	28	31	226.449	3,365	241-C-103
2-Methylhexadecane	1560-92-5	2	0.061	240.476	6.2	241-BY-107
3-Methylhexadecane	6418-43-5	2	0.40	240.476	41	241-BY-107
7,9-Dimethylhexadecane	21164-95-4	3	0.011	254.504	1.1	241-B-103
2,6,10,14-Tetramethylhexadecane	638-36-8	9	0.28	282.558	25	241-BY-110
Heptadecane	629-78-7	20	40	240.476	4,101	241-C-103
3-Methylheptadecane	6418-44-6	1	0.047	254.504	4.5	241-C-110
7-Methylheptadecane	20959-33-5	1	0.46	254.504	44	241-BY-108
8-Methylheptadecane	13287-23-5	1	0.0018	254.504	0.18	241-C-107
2,6,10,14-Tetramethylheptadecane	18344-37-1	1	0.042	296.585	3.5	241-BY-107
2,6,10,15-Tetramethylheptadecane	54833-48-6	1	0.0073	296.585	0.60	241-C-107
9-Octylheptadecane	7225-64-1	1	0.25	352.693	17	241-TY-103
Octadecane	593-45-3	8	0.068	254.504	6.5	241-BY-108
2-Methyloctadecane	1560-88-9	2	0.83	268.531	76	241-TY-103
2,6-Dimethyloctadecane	75163-97-2	1	0.0018	282.558	0.16	241-T-107
Nonadecane	629-92-5	3	0.0027	268.531	0.25	241-C-107
9-Methylnonadecane	13287-24-6	2	0.011	282.558	1.0	241-B-103
Eicosane	112-95-8	6	0.19	282.558	17	241-BY-107
Heneicosane	629-94-7	1	0.012	296.585	1.0	241-C-107
Docosane						
7-Hexyldocosane	55373-86-9	1	0.056	394.774	3.5	241-C-110
Hexacosane	630-01-3	1	0.27	366.720	18	241-BY-108
Summation			1,785		274,443	

Table 2. Cycloalkanes

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
CYCLOALKANES						
Cyclopropane	75-19-4	31	0.55	42.081	320	241-BY-105
Methylcyclopropane	594-11-6	1	0.16	56.108	68	241-C-104
Ethylcyclopropane	1191-96-4	5	6.7	70.135	2,333	241-BY-108
1,1-Dimethylcyclopropane	1630-94-0	4	0.47	70.135	163	241-BY-107
cis-1,2-Dimethylcyclopropane	930-18-7	3	1.1	70.135	370	241-BY-105
trans-1,2-Dimethylcyclopropane	2402-06-4	1	0.045	70.135	16	241-BY-110
Propylcyclopropane	2415-72-7	7	0.60	84.163	173	241-C-102
(1-Methylethyl)cyclopropane	3638-35-5	3	0.27	84.163	77	241-BY-104
Butylcyclopropane	930-57-4	5	2.3	98.190	571	241-BY-108
trans-1-Butyl-2-methylcyclopropane	38851-70-6	1	0.010	112.217	2.2	241-B-103
(1-Methylbutyl)cyclopropane	5458-16-2	1	0.027	112.217	5.8	241-BY-110
Pentylcyclopropane	2511-91-3	3	0.055	112.217	12	241-BY-109
Octylcyclopropane	1472-09-9	2	1.1	154.298	174	241-C-102
1,2-Dibutylcyclopropane	41977-32-6	(a) 1	0.038	154.298	6.1	241-BY-110
1-Pentyl-2-propylcyclopropane	41977-33-7	(a) 1	1.5	154.298	232	241-C-101
1-Ethyl-2-heptylcyclopropane	74663-86-8	(a) 1	0.055	168.325	8.0	241-BY-104
1-Ethyl-2-pentylcyclopropane	62238-08-8	(a) 1	0.0012	140.271	0.21	241-T-107
1,1,2-Trimethyl-3-(2-methylpropyl)cyclopropane	41977-43-9	(a) 1	0.0092	140.271	1.6	241-BY-105
1-Heptyl-2-methylcyclopropane	74663-91-5	(a) 1	0.014	154.298	2.2	241-BY-106
1-Butyl-1-methyl-2-propylcyclopropane	41977-34-8	1	0.0050	154.298	0.80	241-BY-105
1-(2-Butyl)-1-(2-methylbutyl)cyclopropane	UCY012-08	1	0.0060	168.325	0.87	241-TY-104
Cyclobutane	287-23-0	3	0.41	56.108	180	241-BY-107
Methylcyclobutane	598-61-8	1	1.3	70.135	447	241-BY-108
Ethylcyclobutane	4806-61-5	1	0.52	84.163	152	241-BY-107
(1-Methylethyl)cyclobutane	872-56-0	4	0.16	98.190	39	241-BY-106
cis-1,2-Diethylcyclobutane	MCYCY00-01	1	0.42	112.217	92	241-C-102
trans-1,2-Diethylcyclobutane	19341-98-1	2	0.29	112.217	64	241-C-101
1,1,2,3,3-Pentamethylcyclobutane	57905-86-9	1	0.0073	126.244	1.4	241-C-108
Cyclopentane	287-92-3	5	0.60	70.135	208	241-BY-107
Methylcyclopentane	96-37-7	8	1.9	84.163	559	241-BY-108
Ethylcyclopentane	1640-89-7	3	0.037	98.190	9.1	241-BY-104
Dimethylcyclopentane	2452-99-5	(a) 5	0.31	98.190	78	241-S-103
cis-1,2-Dimethylcyclopentane	1192-18-3	3	0.081	98.190	20	241-SX-110
trans-1,2-Dimethylcyclopentane	822-50-4	5	0.45	98.190	112	241-BY-108
cis-1,2-Dimethyl-trans-3-methylcyclopentane	15890-40-1	2	0.032	112.217	7.0	241-SX-114

Table 2. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
cis-1-Ethyl-3-methylcyclopentane	2613-66-3		1	0.0005	112.217	0.12	241-TY-104
cis-1,3-Dimethylcyclopentane	2532-58-3		1	0.0055	98.190	1.4	241-BY-106
trans-1,3-Dimethylcyclopentane	1759-58-6		2	0.016	98.190	4.0	241-SX-111
1,1,3-Trimethylcyclopentane	4516-69-2		2	0.33	112.217	72	241-BY-108
1,2,3-Trimethylcyclopentane	2815-57-8	(a)	1	0.0044	112.217	0.96	241-AX-102
1,2,4-Trimethylcyclopentane	2815-58-9	(a)	1	0.16	112.217	36	241-S-103
a,a,b-1,2,4-Trimethylcyclopentane	4850-28-6		3	0.027	112.217	6.0	241-BY-104
(2-Methylpropyl)cyclopentane	3788-32-7		1	0.023	126.244	4.4	241-TX-118
(1-Methylbutyl)cyclopentane	4737-43-3		2	0.22	140.271	38	241-BY-107
(2-Methylbutyl)cyclopentane	53366-38-4		2	0.32	140.271	56	241-BY-108
1,2-Dimethyl-3-(1-methylethyl)cyclopentane	489-20-3	(a)	2	0.29	140.271	51	241-BY-107
1,3-Dimethyl-2-(1-methylethyl)cyclopentane	32281-85-9	(a)	5	0.70	140.271	121	241-BY-108
1-Methyl-3-(2-methylpropyl)cyclopentane	29053-04-1	(a)	5	0.52	140.271	91	241-BY-108
1-Butyl-2-ethylcyclopentane	72993-32-9	(a)	2	0.10	154.298	16	241-BY-107
1-Butyl-2-propylcyclopentane	62199-50-2	(a)	1	0.15	168.325	21	241-BY-107
1-Hexyl-3-methylcyclopentane	61142-68-5	(a)	6	0.25	168.325	36	241-C-110
1-Hexyl-3,3-dimethylcyclopentane	61142-66-3		1	0.025	180.336	3.4	241-BY-110
1-Pentyl-2-propylcyclopentane	62199-51-3	(a)	4	0.43	182.352	58	241-C-102
Decylcyclopentane	1795-21-7		1	4.9	210.406	565	241-C-103
2-Ethyl-1,1-dimethylcyclopentane	54549-80-3		1	0.0020	126.244	0.39	241-SX-106
cis-1,1,3,4-Tetramethylcyclopentane	53907-60-1		1	0.018	126.244	3.6	241-BY-104
trans-1-Methyl-2-(4-methylpentyl)cyclopentane	66553-50-2		1	0.0005	168.325	0.080	241-TY-104
3-Hexyl-1,1-dimethylcyclopentane	61142-65-2		1	0.0032	182.352	0.43	241-TY-104
Cyclohexane	110-82-7		27	3.9	84.163	1,145	241-C-103
Methylcyclohexane	108-87-2		27	1.5	98.190	365	241-TY-101
Ethylcyclohexane	1678-91-7		5	0.42	112.217	92	241-BY-108
(1-Methylethyl)cyclohexane	696-29-7		1	0.0064	126.244	1.2	241-BY-106
1,1-Dimethylcyclohexane	590-66-9		1	0.0043	112.217	0.94	241-TX-118
1,2-Dimethylcyclohexane	583-57-3	(a)	1	0.23	112.217	50	241-BY-108
cis-1,3-Dimethylcyclohexane	638-04-0		4	0.31	112.217	68	241-BY-108
1,4-Dimethylcyclohexane	589-90-2	(a)	2	0.26	112.217	56	241-C-204
cis-1-Ethyl-2-methylcyclohexane	4923-77-7		1	0.015	126.244	2.8	241-BY-106
Diethylcyclohexane	1331-43-7	(a)	1	0.017	140.271	3.0	241-C-110
Cyclopropylcyclohexane	32669-86-6		3	0.26	124.228	51	241-BY-108
Propylcyclohexane	1678-92-8		3	0.10	126.244	20	241-C-102
1,1,2-Trimethylcyclohexane	7094-26-0		2	1.4	126.244	266	241-C-204

Table 2. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
1,1,3-Trimethylcyclohexane	3073-66-3		9	0.74	126.244	144	241-BY-108
1,2,3-Trimethylcyclohexane	1678-97-3	(a)	2	0.0030	126.244	0.59	241-T-107
a,b,b-1,2,4-Trimethylcyclohexane	7667-60-9		1	0.013	126.244	2.5	241-T-111
a,a,a-1,3,5-Trimethylcyclohexane	1795-27-3		1	0.018	126.244	3.6	241-BY-104
1,3,5-Trimethylcyclohexane	1839-63-0	(a)	2	0.0078	126.244	1.5	241-BY-105
Butylcyclohexane	1678-93-9		4	1.4	140.271	240	241-BY-108
(1-Methylpropyl)cyclohexane	7058-01-7		5	1.9	140.271	336	241-C-103
(2-Methylpropyl)cyclohexane	1678-98-4		1	0.0084	140.271	1.5	241-A-102
cis-1-Ethyl-4-methylcyclohexane	4926-78-7		6	0.52	126.244	101	241-BX-104
trans-1-Ethyl-4-methylcyclohexane	6236-88-0		5	0.16	126.244	30	241-BY-108
1-Methyl-2-propylcyclohexane	4291-79-6	(a)	2	0.071	140.271	12	241-T-111
1-Methyl-3-propylcyclohexane	4291-80-9	(a)	4	0.54	140.271	94	241-C-102
1-Methyl-3-(1-methylethyl)cyclohexane	16580-24-8	(a)	1	0.31	140.271	54	241-C-101
1-Methyl-4-(1-methylethyl)cyclohexane	99-82-1	(a)	2	0.02	140.271	3.7	241-T-111
cis-1-Methyl-4-(1-methylethyl)cyclohexane	6069-98-3		3	0.32	140.271	56	241-BY-108
1,1,2,3-Tetramethylcyclohexane	6783-92-2	(a)	9	0.37	140.271	64	241-C-204
cis-1,1,3,5-Tetramethylcyclohexane	50876-32-9		3	0.42	140.271	74	241-BX-104
trans-1,1,3,5-Tetramethylcyclohexane	50876-31-8	(a)	2	0.019	140.271	3.4	241-C-110
1,1,4,4-Tetramethylcyclohexane	2223-52-1	(a)	1	0.38	140.271	66	241-BY-108
a,a,a,a-1,2,4,5-Tetramethylcyclohexane	61142-24-3		1	0.047	196.379	5.8	241-C-110
1,2,4,5-Tetramethylcyclohexane	2090-38-2	(a)	1	0.0092	140.271	1.6	241-BY-105
(1,2-Dimethylpropyl)cyclohexane	51284-29-8	(a)	1	0.16	154.298	25	241-BY-107
Pentylcyclohexane	4292-92-6		19	2.2	154.298	349	241-C-204
1-Ethyl-2-propylcyclohexane	62238-33-9	(a)	3	0.39	154.298	62	241-BY-108
1,1-Dimethyl-2-propylcyclohexane	81983-71-3		5	0.27	154.298	44	241-C-102
1-Ethyl-2,2,6-trimethylcyclohexane	UCY011-04	(a)	2	0.50	154.298	80	241-BY-108
(3-Methylpentyl)cyclohexane	61142-38-9		1	0.60	168.325	87	241-C-102
(4-Methylpentyl)cyclohexane	61142-20-9		5	2.5	168.325	360	241-BY-108
Hexylcyclohexane	4292-75-5		14	0.61	168.325	89	241-BY-107
1-(1,5-Dimethylhexyl)-4-methylcyclohexane	29799-19-7	(a)	2	0.0025	210.406	0.29	241-C-106
1-Methyl-2-pentylcyclohexane	54411-01-7	(a)	3	0.49	168.325	71	241-BY-108
1-Methyl-3-pentylcyclohexane	54411-02-8	(a)	3	0.071	168.325	10	241-C-110
1-Methyl-4-(1-methylbutyl)cyclohexane	54411-00-6	(a)	4	0.12	168.325	17	241-BY-107
1,2-Diethyl-1-methylcyclohexane	61141-79-5		4	0.33	154.298	52	241-BY-108
1,2-Diethyl-3-methylcyclohexane	61141-80-8	(a)	4	0.43	154.298	68	241-BY-108
2,4-Diethyl-1-methylcyclohexane	61142-70-9		4	0.26	154.298	41	241-BY-107

Table 2. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
1,5-Diethyl-2,3-dimethylcyclohexane	74663-66-4	(a)	2	0.52	168.325	76	241-C-102
(1,2-Dimethylbutyl)cyclohexane	61142-37-8		1	0.0076	168.325	1.1	241-B-103
(2,2-Dimethylcyclopentyl)cyclohexane	61142-23-2		4	0.28	180.336	39	241-BX-104
2-Butyl-1,1,3-trimethylcyclohexane	54676-39-0	(a)	17	3.1	182.352	418	241-C-102
Octylcyclohexane	1795-15-9		6	0.12	196.379	15	241-B-103
1,1,3-Trimethyl-2-(3-methylpentyl)cyclohexane	54965-05-8	(a)	5	0.68	210.406	79	241-BX-104
cis-(1-Cyclohexylmethyl)-2-methylcyclohexane	54824-04-3		1	0.10	194.363	13	241-BY-107
trans-(1-Cyclohexylmethyl)-2-methylcyclohexane	54823-94-8		1	0.23	194.363	29	241-BY-108
cis-(1-Cyclohexylmethyl)-4-methylcyclohexane	66826-95-7		1	0.73	194.363	92	241-BY-108
(2-Ethylcyclohexyl)cyclohexane	13151-74-1		3	0.044	224.433	4.8	241-BY-104
cis-(1-Cyclohexylmethyl)-2-ethylcyclohexane	54934-93-9		3	0.92	208.390	108	241-BY-108
1,3,5-Trimethyl-2-octadecylcyclohexane	55282-34-3	(a)	2	0.13	378.731	8.3	241-BX-104
2-Propyl-1,1,3-trimethylcyclohexane	UCY012-04	(a)	1	0.0055	168.325	0.80	241-BY-106
1,2-Dimethyl-3-pentylcyclohexane	UCY013-03	(a)	1	0.0085	182.352	1.1	241-BY-112
trans-1-(Cyclohexylmethyl)-4-methylcyclohexane	54823-98-2		1	0.0092	194.363	1.2	241-BY-105
cis-1-(Cyclohexylmethyl)-4-ethylcyclohexane	54934-95-1		1	0.0043	208.390	0.51	241-C-109
(1-Propylheptyl)cyclohexane	13151-75-2		1	0.0018	224.433	0.20	241-C-111
Decylcyclohexane	1795-16-0		1	0.0018	224.433	0.20	241-BY-105
2-Cyclohexyloctane	2883-05-8		1	2.4	196.379	297	241-BY-108
Cyclooctane	292-64-8		1	0.0055	112.217	1.2	241-TY-104
Butylcyclooctane	16538-93-5		1	0.30	168.325	44	241-C-102
cis-1,4-Dimethylcyclooctane	13151-99-0		1	0.037	140.271	6.4	241-BY-104
1,5-Dimethylcyclooctane	21328-57-4	(a)	1	0.0092	140.271	1.6	241-BY-105
Cycloundecane							
1,1,2-Trimethylcycloundecane	62376-15-2	(a)	1	0.038	196.379	4.8	241-BY-109
Cyclododecane	294-62-2		7	2.5	168.325	360	241-C-102
Ethylcyclododecane	28981-49-9		1	0.025	196.379	3.1	241-TY-103
Cyclohexadecane	295-65-8		4	0.092	224.433	10	241-S-110
Cyclotetradecane	295-17-0		4	15	196.379	1,826	241-C-103
DECALINS							
Decahydronaphthalene	91-17-8	(a)	2	0.39	138.255	70	241-BY-108
trans-Decahydronaphthalene	493-02-7		13	4.3	138.255	762	241-C-103
trans-2-Methyldecahydronaphthalene	2958-76-1		15	19	152.282	3,091	241-C-103
trans-1,2-Dimethylmethyldecahydronaphthalene	3604-14-6	(a)	1	1.3	166.309	189	241-C-102
trans-1,5-Dimethylethyldecahydronaphthalene	66552-62-3	(a)	3	0.027	166.309	3.9	241-BY-110
trans-1,6-Dimethylethyldecahydronaphthalene	1750-51-2	(a)	5	0.33	166.309	49	241-BY-108

Table 2. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
trans-2,3-Dimethylmethyldecahydronaphthalene	1008-80-6	(a)	7	2.8	166.309	418	241-C-204
trans-2,6-Dimethylmethyldecahydronaphthalene	1618-22-0	(a)	6	2.3	166.309	337	241-C-204
trans-2-Butyl-1-methyldecahydronaphthalene	6305-52-8	(a)	1	0.29	194.363	37	241-BY-108
INDANES							
cis-Octahydro-1H-indene	4551-51-3		1	0.034	124.228	6.7	241-BY-110
trans-2,2,4,4,7,7-Hexamethyloctahydro-1H-indene	54832-83-6		1	0.18	208.390	22	241-BY-107
OTHER BICYCLIC AND TRICYCLIC MOLECULES							
1,1'-Bicyclohexyl	92-51-3		1	0.042	166.309	6.2	241-BY-107
cis-2-Methyl-1,1'-bicyclohexyl	50991-08-7		1	0.11	180.336	15	241-BX-104
trans-2-Methyl-1,1'-bicyclohexyl	50991-09-8		1	0.020	180.336	2.7	241-C-110
Bicyclo[2.2.1]heptane	279-23-2		2	0.17	96.174	44	241-BY-107
Bicyclo[4.1.0]heptane	286-08-8		1	0.021	96.174	5.4	241-C-110
2-Methyl-7-pentylbicyclo[4.1.0]heptane	55937-92-3	(a)	1	1.2	180.336	162	241-C-204
3-Methyl-7-pentylbicyclo[4.1.0]heptane	41977-48-4	(a)	1	0.38	180.336	51	241-BY-108
Bicyclo[2.2.2]octane							
1,2,3,6-Tetramethylbicyclo[2.2.2]octane	62338-45-8	(a)	1	0.055	166.309	8.1	241-C-110
Bicyclo[3.3.1]nonane	280-65-9		1	0.043	124.228	8.5	241-T-111
Summation				115		21,185	
(a) The positional or geometrical isomer has not been defined.							

Table 3. Alkenes

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALKENES						
Ethene						
Cyclooctylethene	61142-41-4	1	0.088	138.255	16	241-BY-107
Propene	115-07-1	30	7.6	42.081	4,421	241-BY-108
2-Methylpropene	115-11-7	49	15	56.108	6,392	241-C-103
1-Cyclohexyl-1-propene	5364-83-0	1	0.92	124.228	180	241-BY-105
1,1`-(1-Methylethylidene)bis-cyclohexane	54934-90-6	1	0.021	208.390	2.5	241-B-103
1,1,3-Trimethyl-3-(2-methyl-2-propenyl)cyclopentane	74421-09-3	(a) 1	0.0092	166.309	1.3	241-BY-105
trans-1-methyl-2-(2-propenyl)cyclopentane	50746-53-7	(a) 1	0.027	124.228	5.4	241-BY-104
1-Butene	106-98-9	26	21	56.108	9,188	241-C-103
2-Methyl-1-butene	563-46-2	3	1.2	70.135	410	241-BY-105
3-Methyl-1-butene	563-45-1	4	1.4	70.135	479	241-BY-108
3,3-Dimethyl-1-butene	558-37-2	1	0.029	84.163	8.5	241-U-106
2,3-Dimethyl-1-butene	563-78-0	1	0.023	84.163	6.7	241-BY-105
2-(Ethyl-1-methylcyclohexyl)-1-butene	74810-42-7	1	0.0018	180.336	0.25	241-BY-106
(2-Ethyl-1-methylbutylidene)cyclohexane	74810-41-6	(a) 1	0.012	180.336	1.6	241-B-103
2-Butene	107-01-7	3	0.85	56.108	372	241-BY-104
2-Methyl-2-butene	513-35-9	3	0.15	70.135	51	241-BY-104
2,3-Dimethyl-2-butene	563-79-1	1	0.12	84.163	35	241-BY-104
E-2-Butene	624-64-6	2	0.12	56.108	52	241-C-104
Z-2-Butene	590-18-1	2	1.5	56.108	639	241-C-103
1-Pentene	109-67-1	15	9.2	70.135	3,196	241-C-103
2-Methyl-1-pentene	763-29-1	5	2.4	84.163	692	241-BY-108
4-Methyl-1-pentene	691-37-2	8	2.3	84.163	666	241-BY-108
3,4-Dimethyl-1-pentene	7385-78-6	2	1.6	98.190	411	241-BY-108
4,4-Dimethyl-1-pentene	762-62-9	2	0.046	98.190	11	241-TX-111
2,2,4-Trimethyl-1-pentene	107-39-1	1	0.017	112.217	3.8	241-T-111
2-Pentene	109-68-2	5	0.87	70.135	304	241-BY-108
2,4-Dimethyl-2-pentene	625-65-0	2	0.034	98.190	8.4	241-B-103
3-Ethyl-2-pentene	816-79-5	1	0.0092	98.190	2.3	241-TY-104
2-Methoxy-2-pentene	61142-47-0	(a) 1	0.0023	100.162	0.56	241-T-107
E-2-Pentene	646-04-8	1	0.65	70.135	227	241-BY-107
E-4-Methyl-2-pentene	674-76-0	1	0.026	84.163	7.5	241-BY-106
Z-2-Pentene	627-20-3	4	1.2	70.135	415	241-BY-108
1-Hexene	592-41-6	14	12	84.163	3,462	241-C-103

Table 3. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
2-Methyl-1-hexene	6094-02-6	1	0.0037	98.190	0.91	241-BY-106
4-Methyl-1-hexene	3769-23-1	1	0.40	98.190	100	241-S-103
5-Methyl-1-hexene	3524-73-0	3	1.5	98.190	365	241-BY-108
4-Ethyl-1-hexene	16746-85-3	1	0.19	112.217	42	241-S-103
3,4-Dimethyl-1-hexene	16745-94-1	4	0.31	112.217	68	241-BY-107
4,5-Dimethyl-1-hexene	16106-59-5	3	0.31	112.217	68	241-BY-108
5,5-Dimethyl-1-hexene	7116-86-1	2	0.016	112.217	3.6	241-C-110
3,4,5-Trimethyl-1-hexene	56728-10-0	1	0.036	126.244	6.9	241-TX-111
3,5,5-Trimethyl-1-hexene	4316-65-8	1	0.0092	126.244	1.8	241-BY-105
2-Hexene	592-43-8	1	0.046	84.163	13	241-BY-104
2,4-Dimethyl-2-hexene	14255-23-3 (a)	1	0.0082	112.217	1.8	241-C-105
E-2-Hexene	4050-45-7	1	0.081	84.163	23	241-BY-104
Z-2-Hexene	7688-21-3	2	0.037	84.163	11	241-BY-105
Z-4,4,5-Trimethyl-2-hexene	55702-61-9	1	0.031	126.244	6.0	241-U-106
Z-3-Hexene	7642-09-3	1	0.021	84.163	6.1	241-BY-105
Z-2,3,4,5-Tetramethyl-3-hexene	60643-93-8	2	0.072	140.271	13	241-C-110
Z-3-Ethyl-2,5-dimethyl-3-hexene	62338-08-3	2	0.26	140.271	45	241-BY-107
1-Heptene	592-76-7	15	1.6	98.190	388	241-BY-108
3-Methyl-1-heptene	4810-09-7	2	0.71	112.217	156	241-BY-108
5-Methyl-1-heptene	13151-04-7	2	0.10	112.217	22	241-BY-109
6-Methyl-1-heptene	5026-76-6	2	0.68	112.217	148	241-BY-108
2,4-Dimethyl-1-heptene	19549-87-2	1	0.11	126.244	21	241-BX-102
2-Heptene	592-77-8	5	0.59	98.190	146	241-BY-105
E-2-Heptene	14686-13-6	4	0.029	98.190	7.3	241-B-103
Z-2-Heptene						
Z-3-Methyl-2-heptene	3404-75-9	1	0.70	112.217	153	241-TX-116
3-Heptene	592-78-9 (a)	1	0.024	98.190	5.9	241-B-103
4-Propyl-3-heptene	4485-13-6	1	0.012	140.271	2.1	241-B-103
Z-3-Heptene	14686-14-7	2	0.021	98.190	5.3	241-BY-104
Z-2,2,3,5,5,6,6-Heptamethyl-3-heptene	54845-26-0	2	0.20	196.379	25	241-C-101
1-Octene	111-66-0	6	0.84	112.217	184	241-BY-108
3-Ethyl-1-octene	74630-08-3	1	0.17	140.271	30	241-S-103
7-Methyl-1-octene	13151-06-9	1	0.020	126.244	3.9	241-C-104
2-Octene	111-67-1 (a)	1	0.68	112.217	148	241-TX-116
E-3-Octene	14919-01-8	1	0.12	112.217	26	241-BY-104

Table 3. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Z-3-Octene	592-98-3		2	0.36	112.217	78	241-BY-108
E-4-Octene	14850-23-8		1	0.0092	112.217	2.0	241-BY-105
1-Nonene	124-11-8		2	0.42	126.244	82	241-BY-108
4-Nonene							
5-Methyl-4-nonene	15918-07-7	(a)	1	0.0027	140.271	0.48	241-BY-106
5-Butyl-4-nonene	7367-38-6	(a)	5	0.13	182.352	17	241-TY-103
E-2-Nonene	6434-78-2		1	0.00060	126.244	0.12	241-TY-104
Z-4-Nonene							
Z-2,3,3-Trimethyl-4-nonene	63830-68-2		3	0.52	168.325	76	241-BY-108
1-Decene	872-05-9		5	0.040	140.271	7.0	241-U-103
4-Methyl-1-decene	13151-29-6	(a)	1	0.0073	154.298	1.2	241-TY-104
5-Methyl-1-decene	54244-79-0		1	0.0017	154.298	0.28	241-TY-104
3,4-Dimethyl-1-decene	50871-03-9		1	0.012	168.325	1.7	241-TY-104
E-2-Decene	20063-97-2		1	0.39	140.271	69	241-C-102
Z-2-Decene							
Z-4-Methyl-2-decene	74630-30-1		2	0.60	154.298	96	241-C-102
3-Decene	19398-37-9	(a)	2	0.14	140.271	24	241-C-101
4-Decene							
7-Methyl-4-decene	UAE011-05	(a)	1	0.0064	182.352	0.86	241-TY-104
E-4-Decene							
E-3-Methyl-4-decene	62338-47-0		1	0.17	154.298	28	241-BY-107
5-Decene	19689-19-1	(a)	1	0.68	140.271	118	241-BY-108
E-5-Decene	7433-56-9		2	0.021	140.271	3.7	241-B-103
1-Undecene	821-95-4		4	0.29	154.298	46	241-BY-108
4-Methyl-1-undecene	74630-39-0		3	1.4	168.325	200	241-BY-108
7-Methyl-1-undecene	74630-42-5		2	0.073	168.325	11	241-C-110
8-Methyl-1-undecene	74630-40-3		1	0.046	168.325	6.7	241-C-110
2-Undecene							
4-Methyl-2-undecene	91695-32-8	(a)	1	0.0032	168.325	0.47	241-TY-104
2,5-Dimethyl-2-undecene	49622-16-4	(a)	1	0.083	182.352	11	241-BY-107
E-2-Undecene							
E-6-Methyl-2-undecene	74630-61-8		1	0.16	168.325	24	241-BY-107
E-7-Methyl-2-undecene	UAE012-03		1	0.075	168.325	11	241-BY-107
E-4,5-Dimethyl-2-undecene	55170-92-8		1	0.010	182.352	1.4	241-U-106
Z-2-Undecene	821-96-5		1	0.00055	154.298	0.087	241-TY-104

Table 3. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Z-8-Methyl-2-undecene	74630-44-7		2	0.35	168.325	51	241-BY-108
3-Undecene							
5-Methyl-3-undecene	UAE012-06	(a)	1	0.0073	168.325	1.1	241-TY-104
8-Methyl-3-undecene	UAE012-04	(a)	1	0.0092	168.325	1.3	241-BY-105
E-3-Undecene	1002-68-2		2	0.021	154.298	3.3	241-T-111
Z-3-Undecene							
Z-2-Methyl-3-undecene	74630-48-1		2	3.0	168.325	439	241-C-102
4-Undecene							
4-Methyl-4-undecene	61142-40-3	(a)	2	1.8	168.325	266	241-C-102
6-Methyl-4-undecene	UAE012-05	(a)	2	0.22	168.325	32	241-BX-104
E-4-Undecene	693-62-9		1	0.0037	154.298	0.58	241-C-107
Z-4-Undecene							
Z-5-Methyl-4-undecene	74630-69-6		1	0.25	168.325	36	241-C-102
5-Undecene	4941-53-1	(a)	10	1.4	154.298	218	241-BY-108
E-5-Undecene	764-97-6		2	1.0	154.298	160	241-C-102
E-7-Methyl-5-undecene	74630-66-3		1	0.68	168.325	99	241-C-102
Z-5-Undecene	764-96-5		1	0.0091	154.298	1.4	241-B-103
Z-7-Methyl-5-undecene	74630-62-9		1	0.10	168.325	15	241-BY-107
1-Dodecene	112-41-4		6	0.39	168.325	57	241-C-102
2-Dodecene							
4-Methyl-2-dodecene	56851-45-7	(a)	1	0.020	182.352	2.7	241-C-110
E-3-Dodecene	7206-14-6		4	0.16	168.325	23	241-TY-103
Z-3-Dodecene	7239-23-8		1	0.27	168.325	40	241-BY-108
4-Dodecene	2030-84-4	(a)	1	0.028	168.325	4.1	241-TY-103
E-4-Dodecene	7206-15-7		2	0.56	168.325	81	241-C-102
Z-5-Dodecene	7206-28-2		1	0.0067	168.325	0.97	241-BY-106
E-6-Dodecene	7206-17-9		1	0.0092	168.325	1.3	241-BY-105
1-Tridecene	2437-56-1		7	0.092	182.352	12	241-C-110
6-Tridecene	24949-38-0	(a)	3	0.10	182.352	14	241-TY-103
7-Methyl-6-tridecene	24949-42-6	(a)	5	2.1	196.379	263	241-BY-108
1-Tetradecene	1120-36-1		4	5.2	196.379	651	241-C-103
E-3-Tetradecene	41446-68-8		3	0.65	196.379	81	241-BY-107
Z-3-Tetradecene	41446-67-7		1	0.23	196.379	29	241-C-110
E-5-Tetradecene	41446-66-6		2	0.58	196.379	72	241-BY-108
Z-6-Tetradecene	41446-61-1		2	0.037	196.379	4.6	241-BY-105

Table 3. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
7-Tetradecene	10374-74-0	(a)	3	0.017	196.379	2.2	241-T-111
Z-7-Tetradecene	41446-60-0		1	0.0023	196.379	0.29	241-TY-104
1-Pentadecene	13360-61-7		4	0.30	210.406	35	241-BY-107
1-Hexadecene	629-73-2		6	2.4	224.433	260	241-C-103
Z-3-Hexadecene	34303-81-6		2	0.037	224.433	4.0	241-BY-104
Z-7-Hexadecene	35507-09-6		3	0.20	224.433	22	241-BY-108
1-Heptadecene	6765-39-5		1	0.0071	238.461	0.73	241-SX-103
1-Octadecene	112-88-9		1	0.0018	252.488	0.18	241-C-111
1-Nonadecene	18435-45-5		1	0.00092	266.515	0.084	241-C-109
E-5-Eicosene	74685-30-6		1	0.62	280.542	54	241-BY-108
CYCLOALKENES							
Cyclohexene	110-83-8		1	0.0092	82.147	2.7	241-BY-105
1-Ethylcyclohexene	1453-24-3		1	0.62	110.201	138	241-C-101
1-Ethyl-6-ethylidenecyclohexane	61141-57-9	(a)	2	0.014	136.239	2.5	241-SX-106
1-Methyl-3-(1-methylethyl)cyclohexene	13828-31-4	(a)	1	0.0049	138.255	0.88	241-TY-104
1-Methyl-4-(1-methylethenyl)cyclohexene	5989-27-5	(a)	1	0.17	136.239	31	241-U-112
1-Methyl-4-(1-methylethenyl)cyclohexene	138-86-3	(a)	2	0.13	136.239	23	241-BX-103
1-Pentylcyclohexene	15232-85-6		2	0.049	152.282	7.9	241-C-110
4-Ethenylcyclohexene	100-40-3	(a)	1	0.0073	108.185	1.7	241-TY-104
cis-1,2-Dimethyl-3-methylenecyclopropane	4866-55-1		1	0.018	82.147	5.5	241-BY-105
1-Butyl-2-ethylcyclopropene	50915-91-8		1	0.015	124.228	2.9	241-BY-106
ALKADIENES							
1,3-Butadiene	106-99-0		14	0.49	54.092	223	241-C-204
2-Methyl-1,3-butadiene	78-79-5		3	0.15	68.120	53	241-BY-104
2,3-Dimethyl-1,3-butadiene	513-81-5		1	0.044	82.147	13	241-BY-106
1,2-Pentadiene	591-95-7		1	0.030	68.120	11	241-BY-105
E-1,3-Pentadiene	2004-70-8						
Z-1,3-Pentadiene	1574-41-0		1	0.077	68.120	28	241-BY-110
2-Methyl-1,3-pentadiene	1118-58-7		4	1.4	82.147	409	241-BY-108
1,3-Pentadiene	504-60-9	(a)	1	0.025	68.120	8.9	241-BY-106
2,3-Dimethyl-1,3-pentadiene	1113-56-0		1	0.010	96.174	2.6	241-TY-104
1,4-Pentadiene	591-93-5						
2,3-Dimethyl-1,4-pentadiene	758-86-1	(a)	1	0.0069	96.174	1.7	241-SX-106
Z-1,3-Hexadiene	592-48-3	(a)	1	0.40	82.145	120	241-BY-105

Table 3. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Z-3-Ethyl-2-methyl-1,3-hexadiene	74752-97-9		1	0.0048	124.228	0.94	241-AX-101
1,4-Hexadiene	592-45-0		3	0.15	82.147	44	241-BY-104
2,3-Dimethyl-1,4-hexadiene	18669-52-8	(a)	1	0.0046	110.201	1.0	241-AX-101
4-Methyl-1,4-hexadiene	1116-90-1	(a)	2	0.027	96.174	7.0	241-BY-104
1,5-Hexadiene	592-42-7	(a)	1	0.11	82.147	33	241-BY-104
2,6-Octadiene	4974-27-0	(a)					
4,5-Dimethyl-2,6-octadiene	18476-57-8	(a)	1	0.026	138.255	4.5	241-BY-109
3,4-Nonadiene	37050-03-6		1	0.44	124.228	87	241-BY-108
4,5-Nonadiene	821-74-9		1	0.55	124.228	108	241-C-102
E,E-4,6-Decadiene							
E,E-3,8-Dimethyl-4,6-decadiene	67730-63-6		2	0.43	166.309	63	241-BY-108
1,11-Dodecadiene	5876-87-9	(a)	1	0.0037	166.309	0.54	241-TY-104
1,12-Tridecadiene	21964-48-7	(a)	1	0.0046	180.336	0.62	241-C-105
Bicyclo[4.2.0]octa-1,3,5-triene	694-87-1		1	0.13	104.153	30	241-C-101
POLYENES							
2,6,10,14,18,22-Tetracosahexaene							
2,6,10,19,23-Pentamethyl-2,6,10,14,18,22-tetracosahexaene	59681-06-0		2	1.0	396.706	62	241-BY-109
2,6,10,15,19,23-Hexamethyl-2,6,10,14,18,22-tetracosahexaene	7683-64-9		1	1.1	410.733	65	241-BY-109
Summation				126		39,460	
(a) The positional or geometrical has not been defined.							

Table 4. Alkynes

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Propyne	74-99-7	5	0.56	40.065	341	241-C-102
1-Nonyne	3452-09-3	1	0.0092	124.228	1.8	241-BY-105
4-Nonyne	20184-91-2	1	0.37	124.228	72	241-BY-108
3-Decyne	2384-85-2	2	0.47	138.255	83	241-BY-108
3-Hexadecyne	61886-62-2	1	0.46	222.418	50	241-C-102
1-Octadecyne	629-89-0	1	0.0018	250.472	0.18	241-T-107
Summation			1.9		548	

Table 5. Benzene, Biphenyl, Napthalene, Fluorene and Their Derivatives

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
BENZENE AND ALKYL BENZENES						
Benzene	71-43-2	69	6.9	78.115	2,152	241-BY-104
Monosubstituted Benzenes						
Methylbenzene	108-88-3	84	4.4	92.142	1,158	241-BX-103
Ethylbenzene	100-41-4	41	0.60	106.169	139	241-BX-103
(1-Methylethyl)benzene	98-82-8	2	0.43	120.196	88	241-C-102
(1-Methylpropyl)benzene	135-98-8	1	0.018	134.223	3.3	241-T-111
Propylbenzene	103-65-1	4	0.026	120.196	5.2	241-C-110
(1,1-Dimethylethyl)benzene	98-06-6	2	0.049	134.223	8.9	241-C-110
(1,1-Dimethylpropyl)benzene	2049-95-8	1	0.017	148.250	2.9	241-T-111
Pentylbenzene	538-68-1	2	1.3	148.250	212	241-C-102
(1-Methylpentyl)benzene	6031-02-3	1	0.82	162.277	123	241-C-102
(1-Methylhexyl)benzene	2132-84-5	1	0.66	176.304	92	241-C-102
(1-Methylheptyl)benzene	777-22-0	1	0.16	190.331	21	241-C-102
(1-Methyldecyl)benzene	4536-88-3	2	0.0055	232.413	0.58	241-C-104
(1-Propylonyl)benzene	2719-64-4	2	0.0046	246.440	0.45	241-C-104
(1-Butylheptyl)benzene	4537-15-9	2	0.0046	232.413	0.48	241-C-104
(1-Pentylheptyl)benzene	2719-62-2	2	0.0064	246.440	0.64	241-C-104
(1-Ethylonyl)benzene	4536-87-2	1	0.0073	232.413	0.77	241-C-105
(1-Butyloctyl)benzene	2719-63-3	1	0.0055	246.440	0.55	241-C-105
(1-Methylundecyl)benzene	2719-61-1	1	0.0046	246.440	0.45	241-C-104
Disubstituted Benzenes						
1,2-Dimethylbenzene	95-47-6	35	0.71	106.169	165	241-BY-108
1,3-Dimethylbenzene	108-38-3	8	0.072	106.169	17	241-U-106
1,4-Dimethylbenzene	106-42-3	17	1.0	106.169	232	241-BY-108
Dimethylbenzene	1330-20-7	(a) 44	1.7	106.169	382	241-BX-103
1-Ethyl-2-methylbenzene	611-14-3	18	0.040	120.196	8.2	241-C-110
1-Ethyl-3-methylbenzene	620-14-4	1	0.036	120.196	7.3	241-SX-107
1-Ethyl-4-methylbenzene	622-96-8	3	0.00049	120.196	0.10	241-TX-118
1-Methyl-2-propylbenzene	1074-17-5	1	0.80	134.223	145	241-C-102
1-Methyl-3-(1-methylethyl)benzene	535-77-3	1	0.013	134.223	2.3	241-T-111
1-Isopropyl-2-methylbenzene	527-84-4	1	0.020	134.223	3.6	241-SX-107
Trisubstituted Benzenes						
1,2,3-Trimethylbenzene	526-73-8	1	0.024	120.196	4.9	241-SX-107
1,2,4-Trimethylbenzene	95-63-6	25	0.074	120.196	15	241-C-107
1,3,5-Trimethylbenzene	108-67-8	22	0.048	120.196	10	241-U-112

Table 5. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
bis-1,1'-(1,4-Butanediyl)benzene	1083-56-3		1	0.012	210.322	1.4	241-TX-105
BIPHENYL							
1,1'-Biphenyl	92-52-4		6	14	154.214	2,180	241-C-103
2-Methyl-1,1'-biphenyl	643-58-3		3	1.6	168.241	240	241-C-102
2,2'-Diethyl-1,1'-biphenyl	13049-35-9		4	0.0025	210.322	0.29	241-TX-105
OTHER ARENES							
Naphthalene	91-20-3		8	0.045	128.175	8.6	241-SX-112
1-Methylnaphthalene	90-12-0		1	0.024	142.202	4.1	241-SX-107
2-Methylnaphthalene	91-57-6		1	0.025	142.202	4.3	241-T-111
1,7-Dimethylnaphthalene	575-37-1		1	0.010	156.229	1.6	241-T-111
2,3-Dimethylnaphthalene	581-40-8		1	0.011	156.229	1.7	241-T-111
(9H)Fluorene	86-73-7		1	0.42	166.225	62	241-C-102
ALKENYLBENZENES							
Benzene							
1-Ethenylbenzene	100-42-5		23	1.2	104.153	280	241-C-103
(1-Methylethenyl)benzene	98-83-9	(a)	3	0.013	118.180	2.7	241-B-103
(1-Propenyl)benzene	637-50-3	(a)	3	0.58	118.180	119	241-C-102
(2-Propenyl)benzene	300-57-2	(a)	2	0.27	118.180	55	241-C-101
(2-Methyl-2-propenyl)benzene	3290-53-7	(a)	1	0.54	132.207	100	241-C-102
Summation				38.4		8,061	
(a) The positional or geometrical has not been defined.							

Table 6. Halogen Containing Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
HALO ALKANES						
Methane						
Chloromethane	74-87-3	37	0.21	50.488	100	241-TX-110
Dichloromethane	75-09-2	60	6.3	84.933	1,815	241-BY-108
Chlorodifluoromethane	75-45-6	8	6.0	86.469	1,685	241-BX-111
Bromomethane	74-83-9	10	0.054	94.939	14	241-U-112
Dichlorofluoromethane	75-43-4	13	0.23	102.924	54	241-AX-102
Trichloromethane	67-66-3	26	0.073	119.378	15	241-TX-105
Dichlorodifluoromethane	75-71-8	41	0.099	120.914	20	241-SX-101
Trichlorofluoromethane	75-69-4	91	166	137.369	29,533	241-BY-104
Tetrachloromethane	56-23-5	38	2.0	153.823	317	241-TX-105
Ethane						
Chloroethane	75-00-3	15	0.10	64.515	39	241-C-107
1,1-Dichloroethane	75-34-3	8	0.044	98.960	11	241-U-112
1,2-Dichloroethane	107-06-2	6	0.049	98.960	12	241-TX-106
1-Chloro-1,1-difluoroethane	75-68-3	17	3.0	100.496	736	241-U-109
1,1,1-Dichloro-1-fluoroethane	1717-00-6	6	0.86	116.951	180	241-S-101
1,1,1-Trichloroethane	71-55-6	27	0.060	133.405	11	241-BY-108
1,1,2-Trichloroethane	79-00-5	12	0.45	133.405	83	241-BY-108
1,1,2,2-Tetrachloroethane	79-34-5	12	0.17	167.850	25	241-BY-108
1,2-Dichloro-1,1,2,2-tetrafluoroethane	76-14-2	10	0.15	170.922	22	241-BY-108
1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	37	0.42	187.376	55	241-TY-104
1,2-Dibromoethane	106-93-4	13	0.077	187.862	10	241-U-112
Propane						
1-Fluoropropane	460-13-9	1	0.15	62.088	58	241-BY-110
1,2-Dichloropropane	78-87-5	5	0.060	112.987	13	241-BY-108
1-Chloro-2,2-dimethylpropane	753-89-9	1	0.016	106.596	3.8	241-U-105
Butane						
1-Chlorobutane	106-97-6					
1-Chlorobutane	109-69-3	6	0.57	92.569	150	241-C-106
2-Bromobutane	78-76-2	2	0.13	137.020	23	241-C-101
Octane						
2-Chlorooctane	628-61-5	1	0.0043	148.678	0.7	241-TX-118
HALO ALKENES						
Ethene						
Fluoroethene	75-02-5	2	0.38	46.045	200	241-C-109

Table 6. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Chloroethene	75-01-4		8	0.028	62.499		
1,1-Dichloroethene	75-35-4		32	0.083	96.944	21	241-S-101
Z-1,2-Dichloroethene	156-59-2		10	0.039	96.944	9.8	241-BY-108
Trichloroethene	79-01-6		18	0.38	131.389	70	241-BY-108
Tetrachloroethene	127-18-4		50	0.71	165.834	104	241-BY-107
Propene							
2-Fluoropropene	1184-60-7		6	1.3	60.072	522	241-BY-108
3-Chloropropene	107-05-1		2	0.020	76.526	6.4	241-U-112
E-1,3-Dichloropropene	10061-02-6		7	0.045	110.971	10	241-BY-108
Z-1,3-Dichloropropene	10061-01-5		8	0.042	110.971	9.2	241-U-112
1,3-Butadiene							
Hexachlorobutadiene	87-68-3	(a)					
AROMATIC HALOGEN COMPOUNDS							
Benzene							
Chlorobenzene	108-90-7		13	0.069	112.560	15	241-BY-108
1,2-Dichlorobenzene	95-50-1		10	0.050	147.005	8.4	241-BY-108
1,3-Dichlorobenzene	541-73-1		15	0.060	147.005	10	241-BY-108
1,4-Dichlorobenzene	106-46-7		17	0.047	147.005	7.8	241-U-112
1,2,4-Trichlorobenzene	120-82-1		10	0.12	181.450	16	241-BY-110
1-Bromo-2-fluorobenzene	1072-85-1		1	0.31	175.000	43	241-U-108
1,1'-Biphenyl							
2-Chloro-1,1'-biphenyl	2051-60-7		5	0.035	188.659	4.5	241-TY-103
3-Chloro-1,1'-biphenyl	2051-61-8		2	0.033	188.659	4.3	241-B-103
4-Chloro-1,1'-biphenyl	2051-62-9		1	0.0026	188.659	0.33	241-TY-104
2,2'-Dichloro-1,1'-biphenyl	13029-08-8		2	0.0057	223.104	0.6	241-BY-112
2,3-Dichloro-1,1'-biphenyl	16605-91-7		1	0.0010	223.104	0.11	241-TY-104
2,5-Dichloro-1,1'-biphenyl	34883-39-1		1	0.00092	223.104	0.10	241-TY-104
2,6-Dichloro-1,1'-biphenyl	33146-45-1		1	0.0032	223.104	0.35	241-TY-104
3,3'-Dichloro-1,1'-biphenyl	2050-67-1		1	0.0069	223.104	0.8	241-TX-118
4,4'-Dichloro-1,1'-biphenyl	2050-68-2		1	0.0038	223.104	0.41	241-TY-104
2,2,4'-Trichloro-1,1'-biphenyl	7012-37-5		1	0.0024	257.549	0.23	241-TY-104
2,4',5'-Trichloro-1,1'-biphenyl	16606-02-3		1	0.0035	257.549	0.33	241-TY-104
2,3,4-Trichloro-1,1'-biphenyl	55702-46-0		1	0.0017	257.549	0.17	241-TY-104
2,3,3',5'-Tetrachloro-1,1'-biphenyl	41464-49-7		2	0.0045	291.994	0.38	241-TY-101
2,3,4',6'-Tetrachloro-1,1'-biphenyl	52663-58-8		2	0.0023	291.994	0.19	241-TX-105

Table 6. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
OTHER							
1,1,1-Trifluoropropanone	421-50-1		1	0.048	112.052	10	241-U-103
1-Butanamine							
1,1,2,2,3,3,4,4,4-Nonafluoro-N-1-butanamine	311-89-7		1	0.076	671.097	2.8	241-C-109
Benzeneethanamine							
N-[Perfluorophenyl]-beta,4-bis[TMSoxy]benzeneethanamine	55429-85-1	(b)	1	0.075	475.611	3.9	241-U-112
Butanamide							
Perfluoro-N-[2-TMSoxy-2-[4-TMSoxy]phenyl]ethylbutanamide	55471-01-7	(b)	1	0.16	493.574	8.2	241-U-106
Silane							
Fluorotrimethylsilane	420-56-4		1	0.0018	92.190	0.49	241-T-107
Summation				191		36,077	
<p>(a) Hexachloro-1,3-butadiene, listed in the first version of this report, has been removed. All positive identifications of this compound have been determined to be suspect, and have been so indicated in the Tank Characterization Database.</p> <p>(b) The trimethylsilyl fragment is designated as TMS in this table.</p>							

Table 7. Alcohols, Phenols, and Ethers

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALKANOLS						
Methanol	67-56-1	66	37	32.042	28,000	241-C-105
Dimethyl-(cyclooctyl)methanol	16624-06-9	1	0.016	170.297	2.4	241-T-111
Phenylmethanol	100-51-6	9	0.045	108.141	10	241-U-106
Phenyl-1,1-dimethylmethanol	617-94-7	5	12	136.195	2,139	241-C-103
Ethanol	64-17-5	77	40	46.070	20,986	241-S-102
2-Butoxyethanol	111-76-2	8	0.29	118.177	61	241-BY-104
2-Tetradecyloxyethanol	2136-70-1	1	1.9	258.448	182	241-BY-108
1-Propanol	71-23-8	71	12	60.097	5,000	241-C-105
2-Methyl-1-propanol	78-83-1	5	0.055	74.124	18	241-TY-104
2,2-Dimethyl-1-propanol	75-84-3	8	7.1	88.151	1,983	241-C-103
1-Cyclopentyl-2,2-dimethyl-1-propanol	UOH010-01	1	0.011	154.240	1.7	241-U-112
2-Propanol	67-63-0	61	4.9	60.097	1,977	241-BY-108
1-(1-Methylethoxy)-2-propanol	3944-36-3	1	0.030	118.177	6.3	241-U-107
2-Methyl-2-propanol	75-65-0	27	0.39	74.124	130	241-BY-105
1-Butanol	71-36-3	89	177	74.124	58,361	241-BY-108
2-Methyl-1-butanol	137-32-6	4	0.15	88.151	41	241-C-101
3-Methyl-1-butanol	123-51-3	2	0.10	88.151	28	241-BX-104
2-Ethyl-1-butanol	97-95-0	1	0.059	102.178	14	241-TY-103
3,3-Dimethyl-1-butanol	624-95-3	3	0.076	102.178	18	241-TX-111
2-Butanol	78-92-2	20	0.62	74.124	206	241-BY-107
2-Methyl-2-butanol	75-85-4	2	0.064	88.151	18	241-BY-104
1-Pentanol	71-41-0	16	0.17	88.151	48	241-BX-104
4-Methyl-2-propyl-1-pentanol	54004-41-0	1	0.032	144.259	5.4	241-TY-103
5-Methoxy-1-pentanol	4799-62-6	1	0.010	118.177	2.1	241-BY-106
2-Pentanol	6032-29-7	2	0.50	88.151	140	241-BY-107
2-Methyl-2-pentanol	590-36-3	5	0.21	102.178	50	241-BY-107
2,3-Dimethyl-2-pentanol	4911-70-0	2	0.0058	116.205	1.2	241-BY-106
3-Ethyl-2-methyl-2-pentanol	19780-63-3	1	0.00092	130.232	0.17	241-T-107
3-Pentanol						
2-Methyl-3-pentanol	565-67-3	3	0.14	102.178	33	241-BY-107
2,3,4-Trimethyl-3-pentanol	3054-92-0	1	0.0092	130.232		
1-Hexanol	111-27-3	14	0.19	102.178	46	241-BX-103
2-Ethyl-1-hexanol	104-76-7	38	1.5	130.232	275	241-C-103
2-Hexanol						
5-Methyl-2-hexanol	627-59-8	1	0.0025	116.205	0.52	241-T-107

Table 7. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
2,3-Dimethyl-2-hexanol	19550-03-9	1	0.00064	130.232	0.12	241-TY-104
3-Hexanol	623-37-0	1	0.034	102.178	8.1	241-U-106
2-Methyl-3-hexanol	617-29-8	1	0.085	116.205	18	241-BY-102
1-Heptanol	111-70-6	14	1.9	116.205	405	241-C-103
2-Heptanol	543-49-7	2	0.25	116.205	52	241-BY-107
2-Methyl-2-heptanol	625-25-2	2	0.0030	130.232	0.57	241-BY-106
3-Ethyl-2-methyl-2-heptanol	19780-59-7	1	0.0063	158.286	0.98	241-BY-112
3-Heptanol	589-82-2	16	0.28	116.205	60	241-BY-107
1-Octanol	111-87-5	15	0.33	130.232	62	241-BY-108
2-Butyl-1-octanol	3913-02-8	5	0.32	186.340	42	241-BY-108
2-Octanol	123-96-6	4	0.38	130.232	71	241-BY-107
2-Methyl-2-octanol	628-44-4	1	0.033	144.259	5.6	241-BY-102
3-Octanol						
6-Ethyl-3-octanol	19781-27-2	1	0.0082	158.286	1.3	241-B-103
3,7-Dimethyl-3-octanol	57706-88-4	1	0.0081	158.286	1.2	241-T-111
1-Nonanol	143-08-8	8	0.022	144.259	3.7	241-BY-102
1-Decanol	112-30-1	2	0.0018	158.286	0.28	241-C-109
2-Ethyl-1-decanol	21078-65-9	1	0.00089	186.340	0.12	241-TY-104
2-Decanol	1120-06-5	1	0.0044	158.286	0.68	241-TY-104
3-Decanol	1565-81-7	1	0.016	158.286	2.5	241-BY-103
5-Decanol	5205-34-5	1	0.023	158.286	3.5	241-B-103
1-Undecanol	112-42-5	1	0.0049	172.313	0.69	241-TX-118
2-Undecanol	1653-30-1	1	0.0032	172.313	0.46	241-TY-104
4-Undecanol	4272-06-4	1	0.0021	172.313	0.30	241-T-107
1-Dodecanol	112-53-8	3	0.0073	186.340	0.96	241-C-104
3-Dodecanol	10203-30-2	1	0.0078	186.340	1.0	241-TY-104
6-Dodecanol	6836-38-0	2	0.013	186.340	1.7	241-B-103
Tridecanol	26248-42-0	(a) 1	0.0089	200.368	1.1	241-T-111
2-Tridecanol	1653-31-2	1	0.0046	200.368	0.56	241-C-105
1-Tetradecanol	112-72-1	2	0.0092	214.395	1.0	241-BY-105
1-Pentadecanol	629-76-5	1	0.019	228.422	2.1	241-TY-101
1-Hexadecanol	36653-82-4	15	10	242.449	1,017	241-C-204
2-Methyl-1-hexadecanol	2490-48-4	1	0.0041	256.476	0.39	241-C-108
1-Heptadecanol	1454-85-9	1	0.021	256.476	2.0	241-BY-110
16-Methyl-1-heptadecanol	41744-75-6	1	0.0037	270.503	0.33	241-C-111
1-Octadecanol	112-92-5	4	11	270.503	994	241-C-204

Table 7. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
1-Nonadecanol	1454-84-8	1	0.0082	284.530	0.71	241-S-105
CYCLOALKANOLS						
Cyclopentanol	96-41-3	5	6.7	86.135	1,900	241-C-103
Cyclohexanol	108-93-0	1	0.0020	100.162	0.49	241-S-111
4-(1,1,3,3-Tetramethylbutyl)cyclohexanol	4631-98-5	1	0.0039	212.379	0.45	241-BY-106
4-Methyl-1-(1-methylethyl)cyclohexanol	470-65-5	(a) 1	0.0012	156.270	0.19	241-TY-104
Cycloheptanol						
1-Methylcycloheptanol	3761-94-2	1	0.00092	128.216	0.17	241-TY-104
4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-ol	13040-03-4	1	0.0055	152.238	0.88	241-C-104
ALKANDIOLS						
1,2-Propanediol	57-55-6	12	0.47	76.096	150	241-A-101
2,3-Butanediol						
2,3-Dimethyl-2,3-butanediol	76-09-5	1	0.0082	118.177	1.7	241-BY-103
3-Hexyne-2,5-diol						
2,5-Dimethyl-2,5-hexyne-2,5-diol	142-30-3	1	0.0021	142.200	0.36	241-TY-104
2,7-Octanediol						
2,7-Dimethyl-2,7-octanediol	19781-07-8	1	0.019	174.286	2.7	241-T-111
1,12-Dodecanediol	5675-51-4	1	0.00092	202.340	0.11	241-C-109
ALKENOLS, ALKENDIOLS, AND ALKYNOLS						
2-Propen-1-ol	107-18-6	2	0.0087	58.081	3.7	241-SX-106
Z-2-Buten-1-ol	4088-60-2	2	0.11	72.108	37	241-C-101
3-Buten-1-ol	627-27-0	2	16	72.108	5,595	241-BY-108
3-Buten-2-ol	598-32-3	7	4.4	72.108	1,492	241-BY-108
1,4-Pentadien-3-ol	922-65-6	1	0.025	84.119	7.2	241-BY-110
5-Hexen-1-ol	821-41-0	1	0.065	100.162	16	241-AX-102
Z-3-Octen-2-ol						
Z-2-Methyl-3-octen-2-ol	18521-07-8	2	0.34	142.243	58	241-C-101
1-Pentyn-3-ol						
3,4-Dimethyl-1-pentyn-3-ol	1482-15-1	1	0.0025	112.173	0.54	241-SX-106
1-Dodecyn-4-ol	74646-36-9	1	0.038	182.309	5.2	241-BY-103
6,10-Dodecadien-1-ol						
3,7,11-Trimethyl-6,10-dodecadien-1-ol	51411-24-6	(a) 1	2.4	224.390	260	241-C-103
1-Tridecyn-4-ol	74646-37-0	1	0.0052	196.336	0.65	241-C-110
Z-9-Octadecen-1-ol	143-28-2	1	0.0046	268.487	0.42	241-C-111
ETHERS						
Dimethyl ether	115-10-6	9	3.8	46.070	2,043	241-C-103

Table 7. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Trimethylene oxide	503-30-0	1	1.3	58.080	560	241-C-105
Ethane						
1,2-Dimethoxyethane	110-71-4	1	0.0092	90.123	2.5	241-BY-105
Propane						
2-Ethoxy-2-methylpropane	637-92-3	1	0.0010	102.178	0.24	241-TY-104
Butane						
1-Methoxybutane	628-28-4	3	1.5	88.151	430	241-BY-105
Dipropylether	108-20-3	1	0.40	102.178	97	241-BY-107
Dibutylether	142-96-1	7	2.1	130.232	396	241-C-103
Pentane						
1-Methoxypentane	628-80-8	1	0.032	102.178	7.7	241-BY-104
E-5-Pentyloxy-2-pentene	56052-85-8	2	0.022	156.270	3.4	241-C-104
Hexane						
3-Methoxyhexane	54658-01-4	2	0.22	116.205	46	241-BY-107
1-Ethoxyhexane	5756-43-4	1	0.10	130.232	19	241-TY-103
Cycloheptane						
Methoxycycloheptane	42604-04-6	2	0.10	128.216	19	241-C-101
trans-1,3-Dimethoxycycloheptane	29887-79-4	1	0.0018	158.243	0.28	241-T-107
Didecylether	2456-28-2	3	0.89	298.557	73	241-BY-108
Divinylether	109-93-3	1	0.089	70.092	31	241-C-107
Diphenylether	101-84-8	2	0.16	170.213	24	241-T-111
Methylphenylether						
1-Butoxy-4-methoxybenzene	20743-95-7	1	0.0037	180.249	0.50	241-C-105
PHENOLS						
Phenol	108-95-2	12	0.080	94.114	21	241-BY-107
2-Methylphenol	95-48-7	2	0.037	108.141	8.3	241-BY-104
3-Methylphenol	108-39-4	2	0.0092	108.141	2.1	241-BY-105
4-Propylphenol	645-56-7	1	0.0028	136.195	0.51	241-SX-103
4-(1,1-Dimethylethyl)phenol	98-54-4	3	0.0012	150.222	0.19	241-C-109
(1,1-Dimethylethyl)-4-methoxyphenol	121-00-6	1	0.0037	180.249	0.50	241-TY-104
2-(1,1-Dimethylethyl)-4-methoxyphenol	25013-16-5	1	0.0027	180.249	0.37	241-BY-106
2,6-bis(1,1-Dimethylethyl)-4-methylphenol	128-37-0	3	4.6	220.358	509	241-C-103
1,3-Benzenediol						
2-Methyl-1,3-benzenediol	608-25-3	1	0.0050	124.141	0.99	241-C-107
4-Hexyl-1,3-benzenediol	136-77-6	1	0.0050	194.276	0.63	241-C-105
Summation			367		136,375	

Table 8. Aldehydes

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALIPHATIC ALDEHYDES						
Ethanal	75-07-0	42	22	44.054	12,000	241-C-105
Propanal	123-38-6	7	0.62	58.081	260	241-C-105
2-Methylpropanal	78-84-2	2	0.010	72.108	3.4	241-S-110
2,2-Dimethylpropanal	630-19-3	1	0.027	86.135	7.8	241-B-103
Butanal	123-72-8	66	19	72.108	6,600	241-C-105
2-Methylbutanal	96-17-3	3	0.073	86.135	21	241-BX-104
3-Methylbutanal	590-86-3	3	0.10	86.135	29	241-B-103
Pentanal	110-62-3	12	0.84	86.135	239	241-C-101
2-Methylpentanal	123-15-9	2	0.21	100.162	51	241-BY-104
3-Methylpentanal	15877-57-3	2	0.17	100.162	43	241-U-111
Hexanal	66-25-1	28	5.2	100.162	1,276	241-C-103
3-Methylhexanal	19269-28-4	3	0.67	114.189	143	241-BY-108
2-Ethylhexanal	123-05-7	2	0.17	128.216	33	241-B-103
Heptanal	111-71-7	25	0.55	114.189	118	241-C-102
Octanal	124-13-0	21	2.4	128.216	455	241-C-103
7-Hydroxy-3,7-dimethyloctanal	107-75-5	1	0.00092	172.270	0.13	241-T-107
Nonanal	124-19-6	25	6.0	142.243	1,040	241-C-103
Decanal	112-31-2	16	0.028	156.270	4.4	241-BY-109
Undecanal	112-44-7	3	0.0037	170.297	0.53	241-C-111
Dodecanal	112-54-9	3	0.0050	184.324	0.67	241-C-111
Tridecanal	10486-19-8	1	0.0018	198.352	0.23	241-C-107
Hexadecanal	629-80-1	1	0.0043	240.433	0.44	241-BY-111
ALKENALS						
Prop-2-enal	107-02-8	1	0.014	56.065	6.0	241-B-103
2-Methylprop-2-enal	78-85-3	3	0.073	70.092	26	241-TY-104
But-2-enal	4170-30-3 (a)	8	0.066	70.092	23	241-C-105
2-Methylbut-2-enal	1115-11-3	1	0.048	84.119	14	241-B-103
Pent-4-enal						
2-Ethylpent-4-enal	5204-80-8	1	0.064	112.173	14	241-BY-104
2-Hexenal	505-57-7	2	0.27	98.146	66	241-C-101
2-Ethyl-2-hexenal	645-62-5 (a)	2	0.11	126.200	21	241-C-105
E-Hex-2-enal	6728-26-3	2	0.28	98.146	71	241-C-101
Z-3-Hexenal	6789-80-6	1	0.019	98.146	4.8	241-U-103
E-2-Heptenal	18829-55-5	2	0.0073	112.173	1.6	241-AX-101
Z-Hept-4-enal	6728-31-0	2	0.0092	112.173	2.0	241-BY-105

Table 8. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Hept-5-enal							
2,6-Dimethylhept-5-enal	106-72-9		1	0.38	140.227	67	241-BY-108
E-2-Octeneal	2548-87-0		1	0.0082	126.200	1.6	241-AX-101
E-Non-2-enal	18829-56-6		3	0.016	140.227	2.9	241-BY-110
E,E-2,4-Nonadienal	5910-87-2		1	0.0049	138.211	0.88	241-AX-101
E-2-Deceneal	3913-81-3		1	0.0039	154.254	0.62	241-AX-101
E,E-Dodecane-7,9-dienal	UAD012-01		1	0.49	180.280	67	241-C-204
Octadec-2-enal	56554-96-2	(a)	2	0.022	266.471	2.0	241-BY-103
2-Dodeceneal	4826-62-4	(a)	1	0.0037	182.309	0.49	241-C-109
CYCLIC COMPOUNDS							
Cyclohexanal							
4-(1-Methylethyl)cyclohexanal	UAD010-02		1	0.019	140.235	3.4	241-C-110
Cyclohex-3-en-1-al							
1,3,4-Trimethylcyclohex-3-en-1-al	40702-26-9	(a)	1	0.0046	152.238	0.74	241-TY-104
AROMATIC ALDEHYDES							
Benzaldehyde	100-52-7		5	0.029	106.125	6.8	241-U-106
Phenoxybenzaldehyde	UAD000-02	(a)	1	0.0027	198.223	0.34	241-C-112
3-Phenoxybenzaldehyde	39515-51-0		1	0.0018	198.223	0.23	241-C-107
Summation				60		22,728	
(a) The positional or geometrical has not been defined.							

Table 9. Ketones

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALIPHATIC KETONES						
2-Propanone	67-64-1	99	46	58.081	19,200	241-C-103
2-Butanone	78-93-3	74	38	72.108	13,055	241-C-103
3-Methyl-2-butanone	563-80-4	17	6.5	86.135	1,848	241-C-103
3,3-Dimethyl-2-butanone	75-97-8	16	0.11	100.162	27	241-TX-110
2-Pentanone	107-87-9	60	4.1	86.135	1,171	241-C-103
3-Methyl-2-pentanone	565-61-7	6	0.15	100.162	36	241-BY-107
4-Methyl-2-pentanone	108-10-1	37	3.8	100.162	940	241-C-103
4,4-Dimethyl-2-pentanone	590-50-1	13	0.13	114.189	27	241-BY-112
3-Pentanone	96-22-0	4	0.038	86.135	11	241-BY-110
2-Methyl-3-pentanone	565-69-5	4	0.055	100.162	13	241-BY-104
2,4-Dimethyl-3-pentanone	565-80-0	1	0.092	114.189	20	241-BY-107
2,2,4-Trimethyl-3-pentanone	5857-36-3	2	0.010	128.216	1.9	241-BY-112
2-Hexanone	591-78-6	59	2.5	100.162	600	241-C-103
4-Methyl-2-hexanone	105-42-0	3	5.0	114.189	1,080	241-C-103
5-Methyl-2-hexanone	110-12-3	7	0.17	114.189	37	241-C-102
6-Methoxy-3-hexanone	29006-00-6	1	0.00060	130.188	0.11	241-TY-104
3-Cyclohexyliden-4-ethyl-2-hexanone	UKE014-03	1	0.25	208.330	29	241-C-102
3-Hexanone	589-38-8	15	26	100.162	6,266	241-C-103
2,5-Dimethyl-3-hexanone	1888-57-9	1	0.030	128.216	5.8	241-AX-102
5-Methyl-3-hexanone	623-56-3	1	0.0081	114.189	1.7	241-AX-102
4-Ethyl-3-hexanone	6137-12-8	1	0.0031	128.216	0.59	241-AX-102
2-Heptanone	110-43-0	58	2.8	114.189	608	241-C-103
3-Methyl-2-heptanone	2371-19-9	3	0.045	128.216	8.6	241-BY-102
4-Methyl-2-heptanone	6137-06-0	5	0.092	128.216	17	241-BY-107
6-Methyl-2-heptanone	928-68-7	30	11	128.216	2,098	241-C-103
4,6-Dimethyl-2-heptanone	19549-80-5	1	0.0056	142.243	1.0	241-BY-112
3-Heptanone	106-35-4	46	8.4	114.189	1,800	241-C-105
6-Methyl-3-heptanone	624-42-0	3	0.027	128.216	5.2	241-BY-104
4-Heptanone	123-19-3	17	2.0	114.189	432	241-C-103
3-Methyl-4-heptanone	15726-15-5	1	0.018	128.216	3.5	241-B-103
2-Octanone	111-13-7	51	1.4	128.216	262	241-C-103
3-Octanone	106-68-3	4	2.3	128.216	437	241-C-103
4-Octanone	589-63-9	7	2.5	128.216	472	241-C-103
3-Methyl-4-octanone	20754-04-5	1	0.016	142.243	2.8	241-AX-102
2-Nonanone	821-55-6	20	9.2	142.243	1,576	241-C-103

Table 9. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
3-Nonanone	925-78-0	1	0.82	142.243	142	241-C-103
4-Nonanone	4485-09-0	3	0.72	142.243	124	241-C-102
5-Nonanone	502-56-7	3	0.014	142.243	2.4	241-BY-104
2-Decanone	693-54-9	8	0.18	156.270	29	241-TY-103
5,9-Dimethyl-2-decanone	33933-82-3	1	0.022	184.324	2.9	241-C-104
4-Decanone	624-16-8	2	0.016	156.270	2.6	241-C-105
5-Decanone	820-29-1	2	0.039	156.270	6.2	241-T-111
2-Undecanone	112-12-9	7	2.6	170.297	369	241-C-103
6,10-Dimethyl-2-undecanone	1604-34-8	1	0.33	198.352	41	241-C-102
3-Undecanone	2216-87-7	6	0.73	170.297	105	241-C-102
4-Undecanone	14476-37-0	1	0.075	170.297	11	241-C-110
5-Undecanone	33083-83-9	4	0.12	170.297	17	241-BX-103
2-Methyl-5-undecanone	50639-02-6	12	1.6	184.324	207	241-C-102
2-Dodecanone	6175-49-1	3	0.13	184.324	17	241-TY-103
3-Dodecanone	1534-27-6	13	8.3	184.324	1,107	241-C-103
4-Dodecanone	6137-26-4	1	0.19	184.324	26	241-BX-103
11-Methyl-4-decanone	29366-35-6	1	0.023	198.352	2.8	241-TY-104
5-Dodecanone	19780-10-0	2	0.20	184.324	27	241-TY-103
6-Dodecanone	6064-27-3	8	0.68	184.324	90	241-TY-103
2-Tridecanone	593-08-8	4	2.0	198.352	249	241-C-101
3-Tridecanone	1534-26-5	18	4.9	198.352	610	241-C-103
4-Tridecanone	26215-90-7	1	0.16	198.352	19	241-BX-103
5-Tridecanone	30692-16-1	4	0.027	198.352	3.4	241-AX-102
6-Tridecanone	22026-12-6	8	0.81	198.352	99	241-TY-103
2-Tetradecanone	2345-27-9	6	0.10	212.379	12	241-TY-103
3-Tetradecanone	629-23-2	3	1.3	212.379	148	241-C-103
4-Tetradecanone	26496-20-8	1	0.012	212.379	1.4	241-TY-104
2-Pentadecanone						
6,10,14-Trimethyl-2-pentadecanone	502-69-2	1	0.0052	268.487	0.48	241-BY-105
2-Heptadecanone	2922-51-2	2	0.00092	254.460	0.088	241-BY-105
ALIPHATIC DIKETONES						
2,3-Pentadione	600-14-6	1	0.064	100.118	16	241-BY-104
2,5-Hexandione	110-13-4	1	0.0071	114.145	1.5	241-AX-102
CYCLOALKANONES						
Cyclobutanone	1191-95-3	1	0.14	70.092	48	241-BY-104
2-Ethylcyclobutanone	10374-14-8	1	0.020	98.146	5.0	241-C-110

Table 9. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
3,3-Dimethylcyclobutanone	1192-33-2	1	0.0043	98.146	1.1	241-TX-118
2,3,3-Trimethylcyclobutanone	28290-01-9	1	0.010	112.173	2.2	241-BY-106
Cyclopentanone						
3-Methylcyclopentanone	1757-42-2	2	0.089	98.146	22	241-C-101
2,4-Dimethylcyclopentanone	1121-33-1	(a) 1	0.024	112.173	5.2	241-C-110
trans-3,4-Dimethylcyclopentanone	19550-73-3	1	0.00055	112.173	0.12	241-TY-104
2,2,5-Trimethylcyclopentanone	4573-09-5	1	0.014	126.200	2.7	241-B-103
2-Methyl-4-(2-methylpropyl)cyclopentanone	69770-96-3	(a) 1	0.43	154.254	68	241-BY-108
Cyclohexanone	108-94-1	22	0.34	98.146	85	241-BY-108
3-Methylcyclohexanone	591-24-2	1	0.019	112.173	4.2	241-T-111
2,6-Dimethylcyclohexanone	16519-68-9	(a) 1	0.0037	154.254	0.58	241-BY-106
4-Hydroxy-4-methylcyclohexanone	17429-02-6	1	0.0018	128.172	0.35	241-C-107
2,2,6-Trimethylcyclohexanone	2408-37-9	2	0.17	140.227	30	241-C-101
3,3,5-Trimethylcyclohexanone	873-94-9	2	0.19	140.227	34	241-C-101
5-Methyl-2-(1-methylethylidene)cyclohexanone	15932-80-6	(a) 1	0.27	152.238	43	241-BY-104
5-Methyl-2-(1-methylethenyl)cyclohexanone	89-82-7	(a) 1	2.3	152.238	368	241-C-204
1,4-Cyclohexanedione	637-88-7	1	0.016	112.129	3.4	241-U-106
Bicyclo[4.1.0]heptan-3-one						
4,7,7-Trimethylbicyclo[4.1.0]heptan-3-one	4176-04-9	1	0.53	152.238	85	241-C-204
ALKENONES						
3-Buten-2-one	78-94-4	19	3.3	70.092	1,151	241-C-103
3-Methyl-3-buten-2-one	814-78-8	2	0.073	84.119	21	241-BY-104
3-Penten-2-one	625-33-2					
4-Methyl-3-penten-2-one	141-79-7	3	0.079	98.146	20	241-AX-102
3-Hexen-2-one	763-93-9	2	0.045	98.146	11	241-AX-102
5-Methyl-3-hexen-2-one	5166-53-0	1	0.016	112.173	3.4	241-AX-102
3-Hepten-2-one	1119-44-4					
3-Methyl-3-hepten-2-one	39899-08-6	(a) 1	0.13	126.200	25	241-AX-102
4-Methyl-3-hepten-2-one	22319-25-1	(a) 1	0.037	126.200	7.1	241-TX-118
4-Hepten-3-one						
5-Ethyl-2,4-dimethyl-4-hepten-3-one	22319-29-5	1	0.21	168.281	31	241-BY-107
5-Hepten-2-one	6714-00-7					
6-Methyl-5-hepten-2-one	110-93-0	1	0.0064	126.200	1.2	241-C-107
1-Octen-3-one	4312-99-6	1	0.031	126.200	6.0	241-BY-106
4-Octen-3-one	14129-48-7	(a) 3	0.018	126.200	3.6	241-BY-104
7-Octen-2-one	3664-60-6	(a) 1	0.0064	126.200	1.2	241-BY-106

Table 9. (contd)

Compound	TCD Identification Number		Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
1-Nonen-3-one							
2-Methyl-1-nonen-3-one	51756-19-5		1	0.0055	154.254	0.87	241-TY-104
2-Nonen-4-one	32064-72-5	(a)	1	0.058	140.227	10	241-U-106
5,9-Undecadien-2-one							
E-6,10-Dimethyl-5,9-undecadien-2-one	3796-70-1		1	0.00064	194.320	0.081	241-AX-103
Z-6,10-Dimethyl-5,9-undecadien-2-one	3879-26-3		3	0.0061	194.320	0.77	241-C-107
2-Pentanone							
4-Cyclohexylidene-3,3-diethyl-2-pentanone	UKE015-01		1	0.16	222.358	17	241-BY-108
10-Undecen-4-one							
2,2,6,6-Tetramethyl-10-undecen-4-one	42565-49-1		1	0.013	224.390	1.4	241-A-102
2-Cyclopenten-1-one							
2,3-Dimethyl-2-cyclopenten-1-one	1121-05-7		1	0.0060	110.157	1.3	241-A-102
3-Cyclopenten-1-one							
2,3,4-Trimethyl-3-cyclopenten-1-one	83321-16-8	(a)	1	0.0041	124.184	0.81	241-TX-118
Cyclohexanone							
2,5-Dimethyl-2-(1-methylethenyl)cyclohexanone	6711-26-8	(a)	1	0.0027	166.266	0.40	241-C-107
2-Cyclohexen-1-one							
4,5-Dimethyl-2-cyclohexen-1-one	5715-25-3	(a)	1	0.023	124.184	4.5	241-BY-102
4-Ethyl-3,4-dimethyl-2-cyclohexen-1-one	17622-46-7	(a)	1	0.0030	152.238	0.49	241-BY-106
3,4-Undecadiene-2,10-dione							
6,6-Dimethyl-3,4-undecadiene-2,10-dione	52588-78-0	(a)	1	0.0018	208.303	0.22	241-BY-106
AROMATIC KETONES AND QUINONES							
1H-Inden-1-one							
2,3-Dihydro-3,3-dimethyl-1H-inden-1-one	26465-81-6		1	0.0027	160.218	0.42	241-C-107
Ethanone							
1-Phenylethanone	98-86-2		19	2.2	120.152	448	241-C-103
1-(2,4,5-Trimethylphenyl)ethanone	2040-07-5		1	0.016	162.234	2.3	241-T-111
1-(3-Methylphenyl)ethanone	585-74-0		1	0.0018	134.179	0.33	241-T-107
1-(5,6,7,8-Tetrahydro-3,5,5,6,8,8-ethanone	1506-02-1	(a)	1	0.00092	258.407	0.087	241-C-109
bis-1,1'-(1,4-phenylene)ethanone	1009-61-6		1	0.0027	162.190	0.41	241-TY-104
1-Propanone							
1-Phenyl-1-propanone	93-55-0		1	0.26	134.179	47	241-C-101
9H-Fluoen-9-one	486-25-9		2	0.016	180.208	2.1	241-C-110
2,5-Cyclohexdiene-1,4-dione							
2,6-bis(1,1-dimethylethyl)-2,5-cyclohexdiene-1,4-dione	719-22-2		8	0.026	220.314	2.9	241-SX-107

Table 9. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Summation			210		58,211	

(a) The positional or geometrical has not been defined.

Table 10. Acids

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALKANOIC ACIDS						
Ethanoic acid	64-19-7	19	0.64	60.053	261	241-C-104
Propanoic acid	79-09-4	4	0.016	74.080	5.1	241-C-108
Butanoic acid	107-92-6	2	3.0	88.107	840	241-C-103
Decanoic acid	334-48-5	2	0.0027	172.270	0.39	241-C-111
Dodecanoic acid	143-07-7	6	0.28	200.324	35	241-BY-108
Tetradecanoic acid	544-63-8	22	3.7	228.378	393	241-C-103
12-Methyltetradecanoic acid	5746-58-7	2	0.0087	242.405	0.88	241-C-107
Pentadecanoic acid	1002-84-2	13	2.2	242.405	222	241-C-103
Hexadecanoic acid	57-10-3	29	3.8	256.432	367	241-C-103
Octadecanoic acid	57-11-4	1	0.0037	284.486	0.32	241-C-108
Cyclohexanecarboxylic acid						
trans-2-(1,1-Dimethylethyl)cyclohexanecarboxylic acid	27392-16-1	1	0.0018	184.281	0.24	241-C-112
ALKENOIC ACIDS						
Propenoic acid	79-10-7	1	4.0	72.064	1,369	241-C-103
Hexenoic acid	142-62-1	1	0.0037	116.161	0.77	241-C-109
2-Ethylhexanoic acid	149-57-5	1	0.0018	144.216	0.31	241-C-109
Pentadec-14-enoic acid	17351-34-7	3	0.038	240.389	3.9	241-BY-107
Hexadec-9-enoic acid	2091-29-4 (a)	14	3.4	254.416	326	241-C-103
Z-Octadec-9-enoic acid	112-80-1	5	0.064	282.470	5.6	241-BY-107
Summation			21		3,829	

(a) The positional or geometrical has not been defined.

Table 11. Esters

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALKANE ESTERS						
Methanoic Acid Ester						
Methyl formate	107-31-3	1	0.0018	60.053	0.75	241-T-107
2-Methylpropyl formate	542-55-2	1	0.27	102.134	66	241-B-103
Vinyl acetate	108-05-4	1	0.0027	86.091	0.78	241-U-112
2-Propenyl formate	1838-59-1	1	3.8	86.091	1,067	241-C-103
Butyl formate	592-84-7	4	3.0	102.134	724	241-C-103
2,6-Dimethylhept-5-en-2-yl formate	UES010-02	3	0.34	170.244	49	241-BY-108
Ethanoic Acid Ester						
Methyl acetate	79-20-9	2	0.13	74.080	42	241-U-103
Ethyl acetate	141-78-6	3	43	88.107	11,957	241-C-103
2-Propenyl acetate	591-87-7	1	4.2	100.118	1,030	241-C-103
Butyl acetate	123-86-4	9	16	116.161	3,280	241-C-103
1-Hepten-1-yl acetate	35468-97-4	1	0.021	156.227	3.3	241-A-103
1-Hexadecyl acetate	629-70-9	3	0.049	284.486	4.3	241-BY-107
Oxoacetic Acid Ester						
Ethyl oxoacetate	6295-06-3	1	0.0013	130.145	0.24	241-AX-103
Propanoic Acid Ester						
2-Propyn-1-yl propionate	1932-92-9	1	0.0055	112.129	1.2	241-U-112
Butyl propionate	590-01-2	1	1.0	130.188	189	241-C-103
Octyl propionate	142-60-9	1	0.027	186.297	3.6	241-U-106
2-Methylpropanoic Acid Ester						
Butyl 2-methylpropionate	97-87-0	1	0.024	144.216	4.0	241-AX-102
1-(1,1-Dimethylethyl)-2-methyl-1,3- propanediyl 2-methylpropionate	74381-40-1	8	0.060	286.415	5.1	241-TY-104
3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropionate	74367-34-3	3	0.0046	216.323	0.52	241-C-109
Butanoic Acid Ester						
1-Methylpropyl butanoate	819-97-6	1	0.00092	144.216	0.16	241-T-107
Butyl butanoate	109-21-7	6	2.4	144.216	404	241-C-103
E-2-Hexenyl butanoate	53398-83-7	1	0.037	170.254	5.3	241-BY-105
Hexyl butanoate	2639-63-6	1	0.00092	172.270	0.13	241-C-109
4-Cyanophenyl butanoate	29052-10-6	1	0.0027	189.216	0.36	241-C-107
Butanedioic Acid Ester						
Diethyl butanedioate	123-25-1	1	4.8	174.198	669	241-C-103
2-Oxo-3-methylpentanoic Acid Ester						

Table 11. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Methyl 2-oxo-3-methylpentanoate	3682-42-6	1	0.021	144.172	3.6	241-U-106
Hexanoic Acid Ester						
Butyl 2-ethylhexanoate	68443-63-0	1	0.010	200.324	1.2	241-AX-102
Pentanoic Acid Ester						
Hexyl pentanoate	1117-59-5	1	0.016	186.297	2.0	241-B-103
Hexandioic Acid Ester						
bis(1-Methylpropyl) hexanedioate	38447-22-2	1	0.0018	258.361	0.17	241-C-107
Dioctyl hexandioate	123-79-5	4	1.5	370.578	97	241-C-103
2-Ethylhexyl hexandioate	4337-65-9	1	0.027	258.361	2.6	241-B-103
bis(2-Ethylhexyl) hexandioate	103-23-1	1	0.059	370.578	3.9	241-S-105
E-Hexa-2-enoic Acid Ester						
(E,E)-2-Hexenyl 2-hexenoate	54845-28-2	1	0.28	196.292	35	241-C-102
4-Methylphenyl 2-hexenoate	69687-91-8 (a)	1	0.012	204.271	1.4	241-U-103
Heptanoic Acid Ester						
Butyl heptanoate	5454-28-4	2	0.0082	186.297	1.1	241-C-105
Tetradecanoic Acid Ester						
1-Methylethyl tetradecanoate	110-27-0	7	1.8	270.459	166	241-C-103
Butyl tetradecanoate	110-36-1	4	2.3	284.486	197	241-C-103
Pentadecanoic Acid Ester						
Butyl pentadecanoate	35996-97-5	1	0.0075	298.514	0.62	241-C-106
Hexadecanoic Acid Ester						
1-Methylethyl hexadecanoate	142-91-6	32	0.40	298.514	33	241-BY-108
2,3-Dihydroxypropyl hexadecanoate	542-44-9	1	0.0037	330.512	0.27	241-C-107
Butyl hexadecanoate	111-06-8	1	0.0024	312.541	0.19	241-C-106
Octadecanoic Acid Ester						
Butyl octadecanoate	123-95-5	1	0.027	340.595	1.9	241-C-105
E-9-Octadecenoic Acid Ester						
Methyl E-9-octadecenoate	1937-62-8	1	0.0078	296.498	0.64	241-C-107
a-Hydroxybenzeneacetic Acid Ester						
Methyl a-hydroxybenzeneacetate	20698-91-3	1	0.0072	166.178	1.1	241-SX-103
Ethyl a-hydroxybenzeneacetate	774-40-3	1	0.013	180.205	1.7	241-SX-106
BENZENE ESTERS						
1,2-Benzenedicarboxylic Acid Ester						
Diethyl phthalate	84-66-2	11	1.2	222.243	131	241-U-106
Dibutyl phthalate	84-74-2	2	0.0055	278.351	0.48	241-C-104

Table 11. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Butyl cyclohexyl phthalate	84-64-0	1	0.073	304.390	5.9	241-S-110
Butyl 2-methylpropyl phthalate	17851-53-5	1	0.010	278.351	0.89	241-C-108
Butyl 2-ethylhexyl phthalate	85-69-8	1	0.0082	334.460	0.60	241-C-104
bis(2-Ethylhexyl) phthalate	117-81-7	1	0.0046	390.568	0.29	241-C-108
4-(1,1-Dimethylethyl)benzoic Acid Ester						
Methyl 4-(1,1-dimethylethyl)benzoate	26537-19-9	1	0.0041	192.260	0.52	241-C-108
PHOSPHATE ESTERS						
Butylphosphoric Acid Ester						
Dibutyl butylphosphate	78-46-6	13	0.71	250.321	70	241-C-103
Phosphoric Acid Ester						
Tributyl phosphate	126-73-8	26	5.9	266.320	539	241-C-103
Summation			93		20,806	

(a) The positional or geometrical isomer has not been defined.

Table 12. Nitriles

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALKANE NITRILES						
Acetonitrile	75-05-8	84	22	41.053	13,000	241-C-103
Hydroxyacetonitrile	107-16-4	1	0.0027	57.052	1.1	241-TY-104
Propanenitrile	107-12-0	66	12	55.080	5,300	241-C-103
2-Methylpropanenitrile	78-82-0	2	0.055	69.107	19	241-BY-104
2,2-Dimethylpropanenitrile	630-18-2	3	0.071	83.134	21	241-TX-111
Butanenitrile	109-74-0	60	7.2	69.107	2,562	241-C-103
Pentanenitrile	110-59-8	57	3.7	83.134	1,078	241-C-103
Hexanenitrile	628-73-9	57	3.4	97.161	854	241-C-103
Heptanenitrile	629-08-3	45	2.9	111.188	645	241-C-103
Octanenitrile	124-12-9	22	1.7	125.215	340	241-C-103
Nonanenitrile	2243-27-8	19	0.84	139.243	148	241-C-103
Decanenitrile	1975-78-6	2	0.010	153.270	1.6	241-U-106
Undecanenitrile	2244-07-7	1	0.0020	167.297	0.29	241-TY-104
Tridecanenitrile	629-60-7	1	0.082	195.351	10	241-BY-107
2,4-Pentadienenitrile	1615-70-9 (a)	1	0.0027	79.102	0.85	241-U-112
ALKENE NITRILES						
2-Propenenitrile	107-13-1	3	0.006	53.064	2.6	241-TX-118
2-Methyl-2-propenenitrile	126-98-7	1	0.10	67.091	37	241-C-101
2-Butenenitrile	4786-20-3 (a)	2	0.016	67.091	5.7	241-C-110
3-Butenenitrile	109-75-1	2	0.057	67.091	21	241-BY-106
CYCLOALKANE NITRILES						
Cyclopropanenitrile	5500-21-0	2	0.020	67.091	7.3	241-C-107
AROMATIC NITRILES						
Benzonitrile	100-47-0	4	0.069	103.125	16	241-C-110
Summation			54		24,071	

(a) The positional or geometrical isomer has not been defined.

Table 13. Amines and Amides

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ALIPHATIC AMINES						
Methanamine						
N, N-Dimethylmethanamine	75-50-3	1	1.6	59.112	645	241-C-103
N-(1-Methylbutylidene)methanamine	22431-09-0	5	0.53	99.177	131	241-BY-107
N-(1-Methylhexylidene)methanamine	22058-71-5	1	0.012	127.231	2.3	241-C-104
N-(4-Hydroxy-2-methoxyphenyl)methanamine	1196-92-5	1	0.019	153.182	3.1	241-SX-106
Propanamine						
3-Cyanopropanamine	151-18-8	1	0.0021	70.095	0.74	241-T-107
2-Hydroxypropanamine	2799-17-9	1	0.58	75.110	190	241-C-105
Butanamine						
N-Ethylidene-1-butanamine	6898-74-4	2	0.032	99.177	7.9	241-U-106
1-Butanone						
4-(Dimethylamino)-1-phenyl-1-butanone	3760-63-2	1	0.015	191.275	1.9	241-C-110
1-Pentanamine						
5-Hydroxy-1-pentanamine	2508-29-4	2	0.0027	103.165	0.65	241-TY-104
1-Octadecanamine						
N,N-Dimethyl-1-octadecanamine	124-28-7	1	0.0037	297.572	0.30	241-TY-104
Ethylenediamine	107-15-3	1	0.56	60.099	230	241-C-105
1,4-Butanediamine	110-60-1	1	0.0011	88.154	0.31	241-TY-104
CYCLIC ALIPHATIC AMINES						
Aziridine						
2-Methylaziridine	75-55-8	3	0.13	57.096	55	241-S-102
2-Ethylaziridine	2549-67-9	5	0.16	71.123	57	241-A-101
Pyrrolidine	123-75-1	2	1.9	71.123	662	241-C-103
4-Piperidinemethanol						
1-Methyl-4-piperidinemethanol	20691-89-8	1	0.039	129.204	7.5	241-U-106
1,3,5,7-Tetraazatri(3.3.1.1(3,7))decane	100-97-0	9	0.029	140.189	5.1	241-TY-101
AROMATIC AMINES						
Benzeneamine						
N-Phenylbenzeneamine	122-39-4	11	0.21	169.228	30	241-BY-108
2-Ethylbenzeneamine	578-54-1	1	0.0076	121.184	1.5	241-A-102
Benzamide						
N-Methylbenzamide	613-93-4	1	0.0018	135.167	0.33	241-C-107
ALIPHATIC AMIDES						
Cyanamide						

Table 13. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Dimethylcyanamide	1467-79-4	1	0.12	70.095	42	241-U-106
Formamide	75-12-7	3	0.008	45.041	4.2	241-BY-112
N-(2-Methylpropyl)formamide	6281-96-5	1	0.024	101.150	5.8	241-BY-106
N-Butylformamide	871-71-6	2	0.055	101.150	13	241-A-101
Acetamide	60-35-5	2	0.0077	59.068	3.2	241-AX-102
N,N-Dimethylacetamide	127-19-5	2	0.046	87.122	13	241-C-105
N-Methylacetamide	79-16-3	1	0.0011	73.095	0.37	241-TY-104
Butanamide	541-35-5	2	0.071	87.122	20	241-AX-102
N-Hexylbutanamide	10264-17-2	1	0.00037	171.285	0.05	241-AX-103
Octanamide						
N-(2-Hydroxyethyl)octanamide	7112-02-9	2	0.026	187.284	3.4	241-A-103
Nonanamide	1120-07-6	1	0.0073	157.258	1.1	241-TY-104
Decanamide						
N-(2-hydroxyethyl)decanamide	7726-08-1	1	0.0050			
Dodecanamide						
N-(2-Hydroxyethyl)dodecanamide	142-78-9	1	0.0071	243.393	0.72	241-TY-104
Hexadecanamide	629-54-9	1	0.0027	255.448	0.26	241-C-108
CYCLIC ALIPHATIC AMIDES						
2-Pyrrolidinone	616-45-5	5	0.88	85.106	253	241-C-103
1-Methyl-2-pyrrolidinone	872-50-4	1	0.10	99.134	25	241-BY-109
2,5-Pyrrolidenedione						
1-Methyl-2,5-pyrrolidione	1121-07-9	2	0.026	113.117	5.5	241-B-103
3-Piperidinecarboxamide						
N-Methyl-3-piperidinecarboxamide	5115-98-0	1	0.0086	142.202	1.5	241-SX-106
Summation			7.2		2,423	

Table 14. Nitrous and Nitric Acid Esters, Nitroso and Nitro Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
NITROUS ACID ESTERS						
Methyl nitrite	624-91-9	13	0.80	61.041	319	241-A-101
Butyl nitrite	544-16-1	5	0.70	103.122	165	241-B-103
NITRATE ESTERS						
Methyl nitrate	598-58-3	13	0.47	77.040	150	241-C-104
Ethyl nitrate	625-58-1	14	1.5	91.067	390	241-C-105
1-Methylethyl nitrate	1712-64-7	4	0.14	105.094	32	241-C-102
Propyl nitrate	627-13-4	21	5.2	105.094	1,200	241-C-105
2-Methylpropyl nitrate	543-29-3	1	0.0020	119.121	0.41	241-TX-105
2,2-Dimethyl-1-propyl nitrate	926-42-1	6	0.16	133.148	29	241-AX-102
Butyl nitrate	928-45-0	19	1.8	119.121	360	241-C-105
3-Methyl-1-butanyl nitrate	543-87-3	5	0.23	133.148	42	241-BX-103
Pentyl nitrate	1002-16-0	11	0.87	133.148	160	241-C-105
Hexyl nitrate	20633-11-8	13	0.57	147.175	94	241-BX-103
Heptyl nitrate	20633-12-9	3	0.036	161.202	5.4	241-TX-111
Nonyl nitrate	20633-13-0	1	0.0013	189.257	0.17	241-TY-104
Decyl nitrate	2050-78-4	1	0.0079	203.284	0.9	241-TX-118
Dinitrate-1,3-propanediol	3457-90-7	1	0.12	166.091	18	241-C-204
Dinitrate-1,4-butanediol	3457-91-8	4	1.9	180.118	261	241-C-103
Dinitrate-1,5-pentanediol	3457-92-9	4	0.026	194.145	3.2	241-B-103
1-Nitrate-1,2,3-propanetriol	624-43-1	1	0.15	137.093	26	241-C-204
1,3-Dinitrate-1,2,3-propanetriol	623-87-0	2	0.077	182.091	10	241-TX-106
NITRO COMPOUNDS						
Methane						
Nitromethane	75-52-5	3	0.13	61.041	51	241-U-112
Trinitrofluoromethane	1840-42-2	2	0.10	12.011	205	241-BX-103
Propane						
1-Nitropropane	108-03-2	2	0.13	89.095	36	241-TY-105
2-Nitro-2-methylpropane	594-70-7	26	0.16	103.122		
2-Methyl-1-nitropropane	625-74-1	1	0.0082	103.122	2.0	241-U-112
Butane						
1-Nitrobutane	627-05-4	5	1.6	103.122	391	241-C-204
2-Nitrobutane	600-24-8	1	0.0050	103.122	1.2	241-U-112

Table 14. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Z-1-Nitropropene	27675-36-1	1	0.0073	87.079	2.1	241-TY-104
Benzene						
Nitrobenzene	98-95-3	2	0.014	123.112	2.7	241-TX-118
1-Nitro-2-methylbenzene	88-72-2	1	0.0078	137.139	1.4	241-TY-104
1-Nitro-3-methylbenzene	99-08-1	1	0.0011	137.139	0.20	241-TY-104
1-Nitro-4-methylbenzene	99-99-0	1	0.0018	137.139	0.33	241-T-107
1-Nitro-4-chlorobenzene	100-00-5	1	0.0049	157.557	0.75	241-C-107
NITROSO COMPOUNDS						
Nitrosomethane	865-40-7	1	0.17	45.041	95	241-TX-118
4-Nitrosomorpholine	59-89-2	1	0.046	116.121	9.7	241-U-108
Methanamine						
N-Methyl-N-nitrosomethanamine	62-75-9	19	0.25	74.083	82	241-U-108
N-Methoxy-N-nitrosomethanamine	16339-12-1	1	0.021	90.082	5.7	241-TX-111
Summation			17		4,153	

Table 15. Heterocyclic Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Oxirane	75-21-8	1	0.048	44.054	26	241-TY-104
Ethyloxirane	106-88-7	1	0.25	72.108	84	241-B-103
Ethenyloxirane	930-22-3	4	2.3	70.092	799	241-BY-108
cis-2-Ethyl-3-propyloxirane	56052-94-9	1	0.15	114.189	31	241-BX-104
(1-Methylbutyl)oxirane	53229-39-3	1	0.0022	114.189	0.47	241-S-111
2-Methyl-2-pentyloxirane	53907-75-8	1	0.015	128.216	2.8	241-C-104
1,3,6-Trioxocane	1779-19-7	1	0.0076	118.134	1.6	241-U-112
Furan	110-00-9	9	8.9	68.076	3,194	241-C-103
2-Methylfuran	534-22-5	2	3.4	82.103	1,010	241-C-103
2-Propylfuran	4229-91-8	2	2.7	110.157	590	241-BY-109
2-Pentylfuran	3777-69-3	2	0.015	138.211	2.6	241-AX-101
2-Heptylfuran	3777-71-7	1	0.30	166.266	44	241-BY-108
2,5-Dimethylfuran	625-86-5	1	0.037	96.130	9.3	241-BY-104
2-Ethyl-5-methylfuran	1703-52-2	2	0.046	110.157	10	241-BY-104
2-Octylfuran	4179-38-8	1	0.0060	180.293	0.81	241-BY-106
2-(2-Methyl-6-oxoheptyl)furan	51595-87-0	1	0.0041	194.276	0.52	241-C-105
2-(3-Oxo-3-phenylprop-1-enyl)furan	717-21-5	1	0.0047	198.223	0.58	241-SX-106
2,3-Dihydrofuran	1191-99-7	5	0.046	70.092	16	241-C-110
3-(1,1-Dimethylethyl)-2,3-dihydrofuran	34314-82-4	1	0.0027	126.200	0.53	241-BY-105
4-(1-Methylpropyl)-2,3-dihydrofuran	34379-54-9	1	0.0050	126.200	0.98	241-AX-102
2,5-Dihydrofuran	1708-29-8	5	5.2	70.092	1,823	241-C-103
Tetrahydrofuran	109-99-9	62	15	72.108	4,973	241-C-103
2,5-Diethyltetrahydrofuran	41239-48-9	(a) 1	0.10	128.216	19	241-A-101
2,5-Dipropyltetrahydrofuran	4457-62-9	(a) 1	0.0062	156.270	0.98	241-TY-104
trans-2,4-Dimethyltetrahydrofuran	39168-02-0	1	0.013	100.162	3.1	241-B-103
Dihydro-2(3H)-Furanone	96-48-0	9	3.2	86.091	911	241-C-103
5-Methyldihydro-2(3H)-furanone	108-29-2	4	0.040	100.118	10	241-AX-102
5-Ethyldihydro-2(3H)-furanone	695-06-7	9	0.082	114.145	17	241-U-106
5-Propyldihydro-2(3H)-furanone	105-21-5	7	0.010	128.172	1.9	241-C-104
5-Butyldihydro-2(3H)-furanone	104-50-7	3	0.0050	142.200	0.87	241-TY-104
5-Hexyldihydro-2(3H)-furanone	706-14-9	2	0.0055	170.254	0.79	241-C-104
3,5-Dimethyldihydro-2(3H)-furanone	5145-01-7	2	0.65	114.145	139	241-C-102
4,4-Dimethyldihydro-2(3H)-furanone	13861-97-7	1	0.0055	114.145	1.2	241-BY-112
5-Ethenyl-5-methyl-2(3H)-furanone	1073-11-6	(a) 1	0.0023	126.157	0.44	241-SX-106
5-Ethyl-5-methyl-2(3H)-furanone	2865-82-9	1	0.0072	128.172	1.4	241-TX-105

Table 15. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
5-Pentyl-2(3H)-furanone	104-61-0	1	0.016	156.227	2.4	241-AX-102
Dihydro-2,5-furandione	108-30-5	1	0.0082	100.075	2.0	241-SX-103
2,4(3H,5H)-Furandione						
3-Methyl-2,4(3H,5H)-furandione	1192-51-4	1	0.016	114.102	3.5	241-AX-102
Tetrahydrofuranmethanol						
trans-5-Methyltetrahydrofuranmethanol	54774-28-6	1	0.0031	116.161	0.66	241-TX-118
Tetrahydrofuranmethanyl acetate	637-64-9	1	0.0027	144.172	0.47	241-T-107
Benzofuranone						
3a,4,5,6-Tetrahydro-3a,6,6-trimethylbenzofuranone	16778-26-0	6	0.67	180.249	91	241-BY-108
Tetrahydrofuranmethanol	97-99-4	1	0.069	102.134	16	241-C-102
Furanacetaldehyde						
alpha-Propylfuranacetaldehyde	31681-26-2	1	0.18	152.195	29	241-BY-107
1,3-Dioxane						
4,4-Dimethyl-1,3-dioxane	766-15-4	1	0.0082	116.161	1.7	241-C-105
1,3-Benzodiox-2-one	20192-66-9	1	0.0021	142.156	0.36	241-C-107
1,4-Dioxane	123-91-1	9	0.29	88.107	81	241-U-111
7-Oxabicyclo[4.1.0]heptane						
1-Methyl-7-oxabicyclo[4.1.0]heptane	1713-33-3	1	0.010	112.173	2.2	241-AX-102
2,3-Dioxabicyclo[2.2.2]oct-5-ene						
1-Methyl-4-(1-methylethyl)-2,3-dioxabicyclo[2.2.2]oct-5-ene	512-85-6	1	13	168.238	1,865	241-C-103
2,2-Bioxepane	74793-02-5	6	0.049	198.308	6.1	241-AX-102
2H-Pyran						
3,4-Dihydro-2-carboxaldehyde-2H-pyran	100-73-2	1	0.0072	112.129	1.6	241-A-102
Tetrahydro-2-(1,1-dimethylethoxy)-2H-pyran	1927-69-1	1	0.0046	158.243	0.71	241-TY-104
2H-Pyran-2-one						
Tetrahydro-5,6-dimethyl-2H-pyran-2-one	24405-16-1	5	1.1	128.172	210	241-BY-108
Tetrahydro-6-hexyl-2H-pyran-2-one	710-04-3	1	0.0025	184.281	0.33	241-S-111
Tetrahydro-6,6-dimethyl-2H-pyran-2-one	2610-95-9	1	0.0027	128.172	0.52	241-C-112
Dihydro-2H-pyran-3(4H)-one	23462-75-1	1	0.0041	100.118	1.0	241-C-107
1H-Imidazole						
2-Methyl-1H-imidazole	693-98-1	1	0.0015	82.106	0.44	241-TY-104
1H-Indole						
2-Phenyl-1H-indole	948-65-2	1	0.0051	193.250	0.65	241-SX-106
1H-Pyrrole	109-97-7	2	0.011	67.091	4.0	241-C-107
2,5-Dimethyl-1H-pyrrole	625-84-3	1	0.010	95.145	2.6	241-SX-106

Table 15. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
1-Pyrrolidinamine						
2-(Methoxymethyl)-1-pyrrolidinamine	59983-39-0	1	0.0016	130.191	0.31	241-TY-104
1-Pyrrolidinecarboxylaldehyde	3760-54-1	1	0.00055	99.134	0.14	241-TY-104
4(3H)-Pyrimidinone	51953-17-4	1	0.020	96.089	5.1	241-BY-102
1H-Pyrrolo(2,3-b)pyridine						
6-Amino-2,3-diphenyl-1H-pyrrolo(2,3-b)pyridine	UHC000-11	1	0.015	285.340	1.3	241-SX-106
Hexahydro-1H-azepin-1-amino						
N-Ethylidenehexahydro-1H-azepin-1-amino	75268-01-8	1	0.0076	140.230	1.3	241-C-112
Pyridine	110-86-1	35	0.39	79.102	122	241-BY-108
2-Methylpyridine	109-06-8	1	0.12	93.129	31	241-C-104
3-Methylpyridine	108-99-6	5	0.14	93.129	36	241-C-101
4-Methylpyridine	108-89-4	5	0.034	93.129	8.9	241-C-105
2-Ethylpyridine	100-71-0	2	0.010	107.156	2.3	241-AX-102
2,4-Dimethylpyridine	108-47-4	4	0.46	107.156	105	241-C-103
2,5-Dimethylpyridine	589-93-5	1	0.082	107.156	19	241-C-104
3,4-Dimethylpyridine	583-58-4	1	0.0065	107.156	1.5	241-S-111
2,6-Dimethylpyridine	108-48-5	1	0.011	107.156	2.5	241-C-104
5-Ethyl-2-methylpyridine	104-90-5	2	0.013	121.184	2.6	241-C-104
2,3,6-Trimethylpyridine	1462-84-6	1	0.00060	121.184	0.12	241-TY-104
1,2,3,6-Tetrahydropyridine	694-05-3	2	0.10	83.134	30	241-U-106
Pyrimidine	289-95-2	3	0.092	80.090	28	241-S-101
4-Methylpyrimidine	3438-46-8	1	0.035	94.117	9.0	241-TX-111
Pyrazine	290-37-9	31	0.39	80.090	119	241-U-102
Methylpyrazine	109-08-0	9	0.021	94.117	5.5	241-TX-111
Ethylpyrazine	13925-00-3	4	0.029	108.144	6.6	241-TX-111
2,3-Dimethylpyrazine	5910-89-4	3	0.014	108.144	3.1	241-A-103
2,5-Dimethylpyrazine	123-32-0	1	0.0017	108.144	0.39	241-S-111
2,5-Dimethyl-3-(3-methylbutyl)pyrazine	18433-98-2	1	0.0092	178.280	1.3	241-C-104
1H-1,2,4-Triazole	288-88-0	2	0.025	69.066	8.8	241-U-103
1-Ethyl-1H-1,2,4-triazole	16778-70-4	1	0.12	97.120	30	241-BY-107
4H-1,2,4-Triazole						
3-Amino-4-ethyl-4H-1,2,4-triazole	42786-06-1	1	0.0087	112.135	1.9	241-C-108
1H-Pyrazole						
1-Methyl-1H-pyrazole	930-36-9	1	0.0060	82.106	1.8	241-TX-118
3-Methyl-1H-pyrazole	1453-58-3	3	0.21	82.106	63	241-BX-104

Table 15. (contd)

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
4,5-Dihydro-1H-pyrazole						
5-Methyl-4,5-dihydro-1H-pyrazole	1568-20-3	1	0.061	84.122	18	241-U-106
4,5-Dimethyl-4,5-dihydro-1H-pyrazole	28019-94-5	1	0.022	98.149	5.5	241-U-106
5-Propyl-4,5-dihydro-1H-pyrazole	75011-90-4	1	0.021	112.176	4.6	241-U-103
4,5-Dihydrooxazole						
2-Methyl-4,5-dihydrooxazole	1120-64-5	6	0.057	85.106	16	241-U-106
2-Propyl-4,5-dihydrooxazole	53833-32-2	3	0.043	139.199	7.6	241-S-102
2-Oxazolidinone						
5-Methyl-3-(2-propenyl)-2-oxazolidinone	55956-20-2	4	0.061	141.171	11	241-U-106
Isothiazole	288-16-4	2	0.0027	85.128	0.79	241-C-112
Benzothiazole	95-16-9	4	0.055	135.189	10	241-BY-106
2-Phenylbenzothiazole	883-93-2	4	0.057	211.287	6.6	241-SX-106
Summation			60		16,780	
(a) The positional or geometrical has not been defined.						

Table 16. Sulfur Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
THIOPHENES						
2-Methoxy-5-methylthiophene	31053-55-1	1	0.021	128.194	4.0	241-C-104
THIOLS						
1-Propanethiol						
2,2-Dimethyl-1-propanethiol	1679-08-9	1	0.28	104.215	67	241-C-105
SULFONES						
Propane						
2-[(1,1-Dimethylethyl)sulfonyl]-2-methylpropane	1886-75-5	3	0.0043	178.295	0.59	241-S-111
Benzene						
Ethylsulfonylbenzene	599-70-2	1	0.081	170.232	12	241-C-109
THIOCARBOXYLIC ACIDS, ESTERS AND AMIDES						
Butanethioic Acid Ester						
S-Decyl ester of butanethiolate	2432-55-5	3	0.22	244.443	22	241-U-106
Benzenesulfonamide						
N-Butylbenzenesulfonamide	3622-84-2	39	1.4	213.301	158	241-BY-108
N-Ethyl-N-methylbenzenesulfonamide	80-39-7	1	0.012	199.273	1.5	241-BY-112
N-Hexylbenzenesulfonamide	7250-80-8	1	0.0043	241.355	0.44	241-C-108
Summation			2.0		264	

Table 17. Silicon Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m ³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
SILANES AND SILOXANES						
Silane						
Trimethylsilane	993-07-7	1	0.040	74.199	13	241-TX-111
Chlorotrimethylsilane	75-77-4	7	0.044	108.644	9.9	241-AX-102
Dimethoxydimethylsilane	1112-39-6	3	0.051	120.225	10	241-S-102
bis(trimethyl)silane						
4,5-Dimethyl-1,4-cyclohexadiene-1,2-diyl) bis(trimethyl)silane	101300-62-3	1	0.0057	252.551	0.55	241-S-111
Heptasiloxane						
Hexadecamethylheptasiloxane	541-01-5	1	0.020	533.159	0.92	241-AX-102
Silanol						
Trimethylsilanol	1066-40-6	7	0.098	90.199	26	241-S-107
Cyclotrisiloxane						
Hexamethylcyclotrisiloxane	541-05-9	50	5.8	222.467	635	241-C-103
Cyclotetrasiloxane						
Octamethylcyclotetrasiloxane	556-67-2	44	4.9	296.622	408	241-C-103
Decamethylcyclotetrasiloxane	141-62-8	1	0.034	310.693	2.7	241-A-103
SILANE ESTERS						
Ethanedioic acid						
bis(TMS) ester of ethanedioic acid	18294-04-7	(a) 4	0.13	234.402	13	241-A-102
Propanedioic acid						
2-(TMSoxy)-bis(TMS) ester of propanedioic acid	38165-93-4	(a) 1	0.010	336.612	0.73	241-AX-102
E-2-Hexenedioic acid						
bis(TMS) ester of E-2-hexenedioic acid	55494-10-5	(a) 1	0.0084	288.495	0.71	241-SX-106
2-[(TMS)oxy]benzoic acid						
TMS ester of 2-[(TMS)oxy]benzoic acid	3789-85-3	(a) 18	0.20	282.491	17	241-A-103
alpha,4-bis(TMSoxy)benzeneacetic acid						
Methyl ester of alpha,4-bis(TMSoxy)benzeneacetic acid	55334-40-2	(a) 2	0.031	326.544	2.3	241-BY-103
TMS ester of alpha,4-bis(TMSoxy)benzeneacetic acid	37148-64-4	(a) 2	0.0064	384.700	0.41	241-C-107
alpha-[(TMS)oxy]benzenepropanoic acid						
TMS Ester of alpha-[(TMS)oxy]benzenepropanoic acid	27750-45-4	(a) 1	0.026	310.545	2.0	241-A-102
OTHER SILICON COMPOUNDS						
2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxa-2,4,5,7-tetrasilaoctane	4342-25-0	1	0.019	294.693	1.6	241-AX-102
1-[4-[(Trimethylsilyl)oxy]phenyl]-1-propanone	33342-89-1	1	0.036	222.362	3.9	241-S-102
Summation			11		1,150	

(a) The trimethylsilyl fragment has been designated as TMS in this table.

Table 18. Other Organic Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
ISOCYANATES						
Methane						
Isocyanatomethane	624-83-9	1	0.042	57.052	18	241-U-106
Propane						
2-Isocyanatopropane	1795-48-8	1	0.040	85.106	12	241-C-110
HYDRAZINES						
Hydrazine						
Methylhydrazine	60-34-4	1	0.0026	46.072	1.4	241-TY-101
1,1-Dimethylhydrazine	57-14-7	4	0.0075	60.099	3.1	241-TX-105
Summation			0.093		34	

Table 19. Inorganic Compounds

Compound	TCD Identification Number	Number of Tanks	Maximum Concentration (mg/m³ at 25 °C)	Molecular Weight (g/mol)	Maximum Concentration (ppbv)	Tank with Maximum Concentration
Hydrogen	1333-74-0	53	107	2.016	1,293,000	241-C-107
Carbon monoxide	630-08-0	17	114	28.011	100,000	241-A-106
Carbon dioxide	124-38-9	76	3,125	44.010	1,737,000	241-B-102
Nitrous oxide	10024-97-2	69	1,979	44.013	1,100,000	241-U-102
Nitric oxide	10102-43-9	37	2.0	30.006	1,600	241-C-103
Nitrogen dioxide	10102-44-0	15	1.1	46.006	600	241-BY-102
Ammonia	7664-41-7	96	726	17.031	1,043,000	241-BY-108
Sulfur oxides	UIN000-01 (a)	1	n.a.	n.a.	370	241-C-104
Carbonyl sulfide	463-58-1	2	0.064	60.075	26	241-TY-101
Carbon disulfide	75-15-0	4	2.5	76.139	795	241-C-103

(a) Because this entry includes various oxides, the molecular weight is ambiguous and the maximum concentration in mg/m³ cannot be calculated.

Table 20. Total Nonmethane Hydrocarbon Measurements and Summations of GC/MS Analyses

Based on TNMHC		Based on SUMMA		Based on TST	
Tank	Maximum Concentration (mg/m ³ at 25 °C)	Tank	Maximum Concentration (mg/m ³ at 25 °C)	Tank	Maximum Concentration (mg/m ³ at 25 °C)
241-C-103	520	241-C-204	220	241-C-103	2100
241-BY-108	310	241-BY-104	210	241-BY-108	580
241-C-204	160	241-BY-108	170	241-C-102	290
241-BX-104	130	241-C-102	130	241-BY-107	170
241-BY-101	57	241-BX-104	110	241-C-101	98
241-BX-103	52	241-TY-103	95	241-BX-104	85
241-TY-103	51	241-C-101	87	241-S-102	68
241-S-102	28	241-BY-107	84	241-TY-103	65
241-BY-102	20	241-BX-103	55	241-BY-101	48
241-TX-111	16	241-BY-110	50	241-BY-104	45

Table 21. Summary of Observations

Category	Total Number of Different Compounds	Total Number of Compounds Observed in Only One Tank	Sum of Maximum Concentration of Compounds (ppmv)	Total Number of Compounds at less than 0.025 mg/m ³	Total Number of Compounds at more than 1000 ppbv	Total Number of Compounds at more than 500 ppbv	Total Number of Compounds at more than 100 ppb
Alkanes	204	51	274	39	33	43	90
Cycloalkanes	155	71	21	43	4	8	36
Alkenes and Alkadienes	169	92	39	55	5	9	39
Alkynes	6	4	0.55	2	0	0	1
Arenes	47	20	8.1	21	3	3	14
Halogen Compounds	61	18	36	17	3	5	10
Alcohols, Phenols and Ethers	119	62	136	59	12	15	25
Aldehydes	46	18	23	21	4	4	9
Ketones	118	59	58	46	11	15	28
Acids	17	5	3.8	8	1	2	7
Esters	54	36	21	28	4	7	12
Nitriles	21	5	24	8	4	6	8
Amines and Amides	38	22	2.4	20	0	2	6
Nitro and Nitroso Compounds	37	15	4.2	13	1	1	10
Heterocycles	98	57	17	54	5	8	13
Sulfur Compounds	8	5	0.26	5	0	0	1
Silicon Compounds	18	9	1.1	7	0	1	2
Miscellaneous Organic Compounds	4	3	0.034	3	0	0	0
Inorganic Compounds	10	1	5,276	0	6	8	9
Total	1,230	553	5,947	449	96	137	320

5.0 Discussion

Organic compounds are ubiquitous in the headspaces of the waste tanks. The alkanes (about 200 compounds), cycloalkanes (about 150 compounds), and alkenes (about 170 compounds) are only modestly more numerous than the other compounds with organic functional groups. There are about 120 ketones; about 120 alcohols, phenols and ethers; and about 100 heterocycles (some of the heterocycles, for example the tetrahydrofurans, could be equally well listed as ethers).

Many semivolatile alkanes and cycloalkanes are recognized as constituents of the hydrocarbon diluents used in various Hanford extraction processes. These diluents are commonly referred to as normal paraffinic hydrocarbon (NPH) in technical reports, but several of the commercial diluents that were actually employed (Vandegrift 1984) were rich in isoparaffins (e.g., 2-methyldodecane and related compounds) or naphthenes (e.g., alkylated cyclopentanes and cyclohexanes).

Virtually all of the other alkanes, alkenes, alkynes, arenes, alcohols and ethers, aldehydes, ketones, acids, esters, amides and amines, nitroso and nitro compounds and nitriles can be accounted for as products of the thermally and radiolytically induced free radical and ionic fragmentation and oxidation reactions of NPH, phosphate esters, and complexants. Most of the heterocycles and miscellaneous compounds can also be accounted for in the same manner. The technical bases for these conclusions are set forth in part in Appendix L of the Organic Solvent Topical Report (Cowley et al. 1998) and in *The Chemistry of Flammable Gas Generation* (Stock 2001) and in *Vapor Chemistry* (Stock 2004).

Few of the molecules containing halogen, silicon, or sulfur atoms can arise from the paraffinic hydrocarbon, phosphate esters or complexants. Some of the analytical observations may be spurious. However, many of the compounds that cannot be directly related to the principal source term arise from other identifiable substances. The bromine- and chlorine-containing compounds presumably arise from tetrabromoethane and the chlorocarbon solvents that were used in operations before 1980 (Klem 1990, Gerber et al. 1992). In addition, the unusual trifluoro ketone listed in Table 6 can be traced to a substance listed by Klem. However, the origins of the freons have not been definitely established. These substances apparently arise from sources other than the liquid and solid wastes. The principal silicon-containing compounds, the bis(trimethylsilyl) derivative of 2-hydroxybenzoic acid and cyclic hexa- and octamethyl siloxane, presumably originate from silicone fluids that were also used in operations (Klem 1990, Gerber et al. 1992). The origin of N-butylbenzenesulfonamide, the most frequently observed sulfur-containing compound, is uncertain. It may be produced from benzenesulfonic acid, a constituent of the resins (Gerber et al. 1992) used during operations.

In summary, a broad array of inorganic and organic vapors has been observed in the high-level waste single-shell tank headspaces. These vapors and their highest reported concentrations have been tabulated by functional group and concentration in this report.

6.0 References

- Bolling SD. 2002a. *WSCF Analytical Laboratory Report Industrial Hygiene Analysis for CH2M-Hill Group*, Group#: 20021157. Report Date 16-Oct-2002, Fluor Hanford, Inc., Richland, Washington.
- Bolling SD. 2002b. *WSCF Analytical Laboratory Report Industrial Hygiene Analysis for CH2M-Hill Group*, Group#: 20021190. Report Date 11-Nov-2002, Fluor Hanford, Inc., Richland, Washington.
- Bolling SD. 2003a. *WSCF Analytical Laboratory Report Industrial Hygiene Analysis for CH2M-Hill*, Group#: 20021268, Report Date 25-Mar-2003, Fluor Hanford, Inc., Richland, Washington.
- Bolling SD. 2003b. *WSCF Analytical Laboratory Report Industrial Hygiene Analysis for CH2M-Hill*, Group#: 20021267, Report Date 31-Mar-2003, Fluor Hanford, Inc., Richland, Washington.
- Bolling SD. 2003c. *WSCF Analytical Laboratory Report Industrial Hygiene Analysis for CH2M-Hill*, Group#: 20021651, Report Date 17-Apr-2003, Fluor Hanford, Inc., Richland, Washington.
- Bolling SD. 2004. *WSCF Analytical Laboratory Report Industrial Hygiene Analysis for CH2M-Hill*, Group#: 20040085, Report Date 27-Apr-2004, Fluor Hanford, Inc., Richland, Washington.
- Cowley WL, JE Meacham, JM Grigsby, and AK Postma. 1998. *Organic Solvent Topical*, HNF-SD-WM-CN-032 Rev. 1, Duke Engineering and Services, Inc., Richland, Washington.
- Gerber MA, LL Burger, DA Nelson, JL Ryan, and RL Zollars. 1992. *Assessment of Concentration Mechanisms for Organic Wastes in Underground Storage Tanks at Hanford*, PNL-8339, Pacific Northwest National Laboratory, Richland, Washington.
- Huckaby JL, H Babad, and DR Bratzel. 1995. *Headspace Gas and Vapor Characterization Summary for the 43 Vapor Program Suspect Tanks*, WHC-SD-WM-ER-514, Rev. 1, Westinghouse Hanford Company, Richland, Washington.
- Huckaby JL, JA Edwards, JC Evans, JS Fruchter, JL Julya, KB Olsen, KH Pool, BL Thomas, KL Silvers, L Jensen, LL Buckley, SR Wilmarth, and LD Pennington. 1996. *Comparison of Vapor Sampling System (VSS) and In Situ Vapor Sampling (ISVS) Methods on Tanks C-107, BY-108, and S-102*, PNNL-11186 Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.
- Huckaby JL, JC Evans, DS Sklarew, and AV Mitroshkov. 1998. *Waste Tank Ventilation Rates Measured with a Tracer Gas Method*, PNNL-11925, Pacific Northwest National Laboratory, Richland, Washington.
- Klem MJ. 1990. *Inventory of Chemicals Used at Hanford Site Production Plants and Support Operations (1944-1980)*, WHC-EP-0172, Revision 1, Westinghouse Hanford Company, Richland, Washington.

Pacific Northwest National Laboratory (PNNL). 2004. *Tank Characterization Database*, Version 3.24, Pacific Northwest National Laboratory, Richland, Washington.

Stock LM and JL Huckaby. 2000. *A Survey of Vapors in Headspaces of Single-Shell Waste Tanks*, PNNL-13366, Pacific Northwest National Laboratory, Richland, Washington.

Stock LM. 2001. *The Chemistry of Flammable Gas Generation*, RPP-6664, Rev.1, CH2M Hill Hanford Group, Richland, Washington.

Stock LM. 2004. *Occurrence and Chemistry of Organic Compounds in Hanford Site Waste Tanks*, RPP-21854, Rev. 0, CH2MHill Hanford Group, Inc., Richland, Washington.

TWINS (Tank Waste Information Network System). 2004.

[http://twins.pnl.gov/dictionary/FieldHelp.asp?source=vapor.dbo.sp WEB TVD analysis results.](http://twins.pnl.gov/dictionary/FieldHelp.asp?source=vapor.dbo.sp_WEB_TV_D_analysis_results)

Accessed July 2004.

Vandegrift GF. 1984. *Diluents for the TBP Extraction Systems, in Science and technology of Tributyl Phosphate*, Volume I, Edited by WW Schultz and JD Navratil, CRC Press, Boca Raton, Florida.

Distribution

No. of Copies		No. of Copies	
4	DOE Richland Operations Office		
	R. C. Barr	H6-60	T. A. Hu
	D. C. Bryson	H6-60	M. T. Hughey
	D. L. Noyes	H6-60	J. W. Jabara
	J. H. Swailes	H6-60	L. L. Johns-Andersch
			N. W. Kirch
			M. R. Koch
			M. F. Marcus
39	CH2M HILL Hanford Group, Inc.		G. L. McLellan
	D. I. Allen	H6-03	J. E. Meacham
	T. J. Anderson	R2-50	R. Ni
	S. A. Barker	S5-24	R. S. Popielczyk
	W. B. Barton	R2-11	R. E. Raymond
	S. J. Bensussen	H6-18	D. A. Reynolds
	R. J. Cash	H6-03	A. Sastry
	W. L. Cowley	R1-44	J. S. Schofield
	G. Crawford	R3-86	M. Stauffer
	E. J. Cruz	R3-86	M. L. Zabel
	C. DeFig-Price	R2-58	
	J. A. Eacker	R2-50	17 Pacific Northwest National Laboratory
	S. J. Eberlein	H6-03	J. C. Evans
	M. W. Elkins	R1-06	J. L. Huckaby (10)
	J. G. Field	H6-62	G. B. Josephson
	K. A. Gasper	H6-03	L. A. Mahoney
	D. C. Hedengren	R3-73	D. S. Sklarew
	R. L. Higgins	R2-50	C. W. Stewart
	J. O. Honeyman (5)	H6-03	Hanford Technical Library (2)
			S5-08
			S7-83
			S7-83
			S7-83
			R2-58
			S7-70
			H6-07
			R3-86
			R2-58
			H6-03
			H6-03
			H6-03
			S7-90
			H6-07
			S7-12
			S3-30
			R1-06
			K6-96
			K7-15
			K9-69
			K7-15
			K6-96
			K7-15
			P8-55