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Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

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

L. M. Stock
J. L. Huckaby

October 2000

Prepared for the U.S. Department of Energy
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Contents

Tables

Introduction

This report summarizes data on the organic vapors in the single-shell, high-level radioactive waste tanks at the Hanford Site to support a forthcoming toxicological study. All data were obtained from the Tank Characterization Database (TCD) (PNNL 1999). The TCD contains virtually all the available tank headspace characterization data from 1992 to the present, and includes data for 109 different single-shell waste tanks. 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. This is a revision of a report issued on March 1, 2000 (Stock and Huckaby 2000).

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^{TM} 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.[1] Samples from each of these 104 tanks were analyzed using gas chromatograph/ mass spectrometer (GC/MS) systems, with robust methods that were designed to maximize the number and types of species that could be detected. This summary report includes GC/MS results from about 1,200 tank headspace samples.

Sampling and analysis plans specified that samples be analyzed for as many as 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 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. 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 only considered to be accurate to a factor of 2.

[1] 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/m^3.

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,[2] and the reported concentrations should be assumed to vary accordingly.

The TCD contains about 35,000 results for compounds detected by GC/MS organic vapor analyses. This report summarizes the results for about 1,200 compounds, of which about 500 were found in only one type of sample from a single tank. About 430 of the 1,200 compounds have maximum reported concentrations of less than 0.025 mg/m^3. Suspect results (flagged by the analyst as suspect or associated with blank contamination) and results for ambiguously identified species (e.g., species identified as "unknown", "unknown C-12 alkanone", etc.) were not included in this report.

Procedure

Results for 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 those 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 6a) and not in the alkene table (Table 3a).

Because these tables were prepared primarily for the assessment of toxicological hazards, each table is divided into two parts based on whether the highest reported concentration of the compound is above 0.025 mg/m^3 (about 5 ppbv). Tables 1a, 2a, etc., contain those compounds that have reported maximum concentrations at or above 0.025 mg/m^3, and Tables 1b, 2b, etc., contain those compounds that have reported maximum concentrations below 0.025 mg/m^3. The 0.025 mg/m^3 threshold value was recommended by Bartley (1999) as appropriately conservative in their evaluation of the toxicological hazards associated with the organic vapors emanating from tank C-106 during sluicing operations.

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.

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[2] 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 are actively ventilated. Passive ventilation rates are discussed by Huckaby et al. 1998.

In some instances two or more compounds coelute chromatographically. The identification of coeluting compounds presents a significant analytical challenge, and these observations were treated in the following manner. Insofar as possible, these observations were included. For example, after the numerous entries for decane in the database, there appears the entry "decane and others" at 0.036 mg/m^3. Results of this kind were counted as an observation for the identified compound, i.e., decane. As another example, after the numerous entries for dodecane in the database, there appears the entry "dodecane and 2'-hydroxy-5'-methoxyacetophenone" at 0.095 mg/m^3. This result was included as an observation for dodecane, but the observation for the acetophenone was not included, since it had not been observed independently.

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 1a to 18a, and 1b to 18b. 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 of analytical observations for the compound, the maximum observed concentration in mg/m^3, 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.

Supplementary information about the concentrations of the organic compounds in the tank headspaces is provided in Table 20. This table, 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 non-methane hydrocarbon (TNMHC) measurement was conducted by analysis of Summa 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 Summa and TST samples are also given.

Finally, Table 21 provides a summary of the results. This table provides perspective on the relationship between the total number of different compounds listed in the category with the number of compounds in the same category that have been observed only once or more than once at a concentration less than 0.025 mg/m^3. The table lists the sum of the maximum concentration of the compounds in the category in ppbv. 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.

Discussion

Organic compounds are ubiquitous in the headspaces of the waste tanks. The alkanes (about 200 compounds), cycloalkanes (about 150 compounds), and alkenes (about 150 compounds) are only modestly more numerous than the other compounds with organic functional groups. There are about 120 ketones, about 110 alcohols, phenols and ethers and about 100 heterocycles (some of the heterocycles, for example the tetrahydrofurans, could be equally well listed as ethers).

The sum of the maximum concentrations of the 1,200 organic compounds is about 630 ppmv. The alkanes contribute about 250 ppmv, the alcohols and ethers contribute about 120 ppmv (not including the heterocyclic ethers), and the ketones contribute about 60 ppmv. The sum of the maximum concentrations of the halogen compounds is also significant at about 40 ppmv.

Many semivolatile alkanes and cycloalkanes are recognized as constituents of the normal paraffinic hydrocarbon (NPH) diluent used in various Hanford extraction processes. 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 2000).

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 and butyl amine generated in ammonia-rich waste.

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.

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Tables of Maximum Tank Headspace Vapor Concentrations

Table 1a. Alkanes (Page 1 of 3)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
Propane	62	1.600	44	815	BY-107
2-Methyl-	22	1.700	58	657	BY-106
2,2-Dimethyl-	5	0.013	72	4	U-107
Butane	141	20.000	58	7724	C-103
2-Methyl-	13	7.900	72	2458	BY-108
2,2-Dimethyl-	9	0.140	86	36	U-107
2,3-Dimethyl-	1	0.032	86	8	U-107
2,2,3-Trimethyl-	1	0.100	100	22	TY-104
2,2,3,3-Tetramethyl-	3	0.240	114	47	BX-111
Pentane	117	6.500	72	2022	BY-108
2-Methyl-	36	15.000	86	3907	BY-108
3-Methyl-	24	2.500	86	651	BY-108
3-Ethyl-	3	0.970	100	217	TY-104
2,2-Dimethyl-	1	0.051	100	11	TY-104
2,3-Dimethyl-	21	3.200	100	717	TY-101
2,4-Dimethyl-	7	0.550	100	123	U-102
3,3-Dimethyl-	19	1.400	100	314	TY-101
3-Ethyl-2-methyl-	1	0.024	114	5	BY-106
2,3,3-Trimethyl-	4	1.300	114	255	TX-116
2,3,4-Trimethyl-	1	0.290	114	57	TX-116
Hexane	146	8.600	86	2240	BY-108
2-Methyl-	21	3.700	100	829	TY-101
3-Methyl-	32	5.600	100	1254	TY-101
2,3-Dimethyl-	3	1.100	114	216	BY-107
2,4-Dimethyl-	11	1.700	114	334	BY-108
2,5-Dimethyl-	5	0.230	114	45	AX-102
2,2,5-Trimethyl-	3	0.060	128	11	SX-107
2,3,5-Trimethyl-	7	0.300	128	53	BX-103
2,2,5,5-Tetramethyl-	1	0.026	142	4	U-106
3,3,4,4-Tetraethyl-	1	0.082	142	13	BY-107
Heptane	165	4.400	100	986	BY-108
2-Methyl-	9	2.000	114	393	BY-108
3-Methyl-	15	0.560	114	110	BY-108
3-Ethyl-	2	0.038	128	7	T-111
4-Methyl-	2	2.000	114	393	C-103
2,3-Dimethyl-	6	0.280	128	49	BY-108
2,4-Dimethyl-	10	0.670	128	117	BY-101
2,5-Dimethyl-	3	0.110	128	19	TX-116
2,6-Dimethyl-	8	0.550	128	96	BY-108
3,5-Dimethyl-	1	0.220	128	39	BY-108
2,2,4-Trimethyl-	4	0.660	142	104	TX-116
2,3,5-Trimethyl-	1	1.900	142	300	BY-108
2,3,6-Trimethyl-	2	1.900	142	300	BY-108
3,3,5-Trimethyl-	4	0.230	142	36	AX-104
2-Methyl-3-ethyl-	7	0.073	142	12	BY-104
2-Methyl-5-ethyl-	1	0.045	142	7	BY-102
5-Methyl-3-ethyl-	2	1.100	142	174	C-102
4-(1-methylethyl)-	2	0.440	170	58	BY-108
4-Ethyl-2,2,6,6-tetramethyl-	2	0.370	184	45	AX-104
2,2,3,4,6,6-Hexamethyl-	4	0.240	184	29	B-103
Octane	137	1.800	114	354	C-103
3-Methyl-	6	0.620	128	109	BY-108
4-Methyl-	6	1.200	128	210	C-102
4-Ethyl-	2	0.070	142	11	BY-109
2,5-Dimethyl-	2	0.330	142	52	C-101
2,6-Dimethyl-	6	0.330	142	52	BY-107
3,5-Dimethyl-	2	0.160	142	25	BY-104
2,3,3-Trimethyl-	1	0.700	156	101	BY-107
2,3,7-Trimethyl-	4	3.100	156	445	BX-104
2,5,6-Trimethyl-	2	0.031	156	4	U-107
2-Methyl-5-ethyl-	1	0.180	156	26	C-101
2-Methyl-6-ethyl-	5	0.290	156	42	BY-108

Table 1a. Alkanes (Page 2 of 3)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
Nonane	141	1.700	128	298	C-103
2-Methyl-	2	0.130	142	21	BY-107
3-Methyl-	3	0.240	142	38	BY-108
4-Methyl-	11	0.710	142	112	C-102
2,6-Dimethyl-	2	4.200	156	603	C-103
4,5-Dimethyl-	2	0.009	156	1	BY-105
3,7-Dimethyl-	6	2.400	156	345	BY-108
3-Methyl-5-propyl-	6	0.660	184	80	U-106
5-(2-Methylpropyl)-	2	0.057	184	7	BY-110
5-Butyl-	4	0.340	184	41	BY-107
Decane	147	18.000	142	2839	C-103
2-Methyl-	16	2.100	156	302	C-102
3-Methyl-	9	1.100	156	158	C-102
4-Methyl-	16	1.000	156	144	C-204
5-Methyl-	5	0.890	156	128	C-102
5-Propyl-	3	0.028	184	3	T-107
2,5-Dimethyl-	3	3.200	170	422	C-101
2,9-Dimethyl-	2	0.014	170	2	A-102
3,8-Dimethyl-	5	0.300	170	40	BX-104
2,2,8-Trimethyl-	2	0.280	184	34	U-106
2,3,5-Trimethyl-	3	0.230	184	28	BY-109
2,3,6-Trimethyl-	6	0.710	184	86	BY-108
2,3,7-Trimethyl-	3	1.000	184	122	BX-104
2,3,8-Trimethyl-	4	0.260	184	32	BY-107
2,4,6-Trimethyl-	3	24.000	184	2922	C-103
2,5,9-Trimethyl-	1	0.029	184	4	BY-109
2,6,7-Trimethyl-	4	1.400	184	170	BY-104
2,6,8-Trimethyl-	2	0.014	184	2	TY-104
2-Methyl-6-ethyl-	1	2.200	184	268	C-102
2,3,5,8-Tetramethyl-	1	0.160	198	18	BY-108
Undecane	156	92.000	156	13210	C-103
2-Methyl-	16	28.000	170	3689	C-103
3-Methyl-	14	18.000	170	2372	C-103
4-Methyl-	19	13.000	170	1713	C-103
5-Methyl-	14	6.900	170	909	C-103
5-Ethyl-	5	1.300	184	158	C-102
6-Methyl-	10	3.500	170	461	C-102
2,3-Dimethyl-	3	0.970	184	118	BY-108
2,4-Dimethyl-	10	15.000	184	1826	C-103
2,5-Dimethyl-	1	0.099	184	12	C-110
2,6-Dimethyl-	29	41.000	184	4991	C-103
2,7-Dimethyl-	2	0.600	184	73	BY-108
2,8-Dimethyl-	4	0.850	184	103	BY-107
2,9-Dimethyl-	2	0.240	184	29	BY-107
2,10-Dimethyl-	14	39.000	184	4748	C-103
3,4-Dimethyl-	3	0.710	184	86	TY-103
3,6-Dimethyl-	2	0.100	184	12	BY-107
3,7-Dimethyl-	9	22.000	184	2678	C-103
3,8-Dimethyl-	5	4.200	184	511	C-102
3,9-Dimethyl-	2	0.190	184	23	A-106
4,4-Dimethyl-	4	0.570	184	69	TY-103
4,6-Dimethyl-	3	5.200	184	633	C-101
4,7-Dimethyl-	4	2.300	184	280	BY-108
4,8-Dimethyl-	5	0.500	184	61	C-102
5,5-Dimethyl-	1	1.400	184	170	BX-104
5,7-Dimethyl-	3	0.810	184	99	TY-103
6,6-Dimethyl-	1	0.890	184	108	BY-108
Dodecane	156	388.00	170	51125	C-103
2-Methyl-	3	3.000	184	365	C-102
3-Methyl-	5	1.800	184	219	C-102
4-Methyl-	15	19.000	184	2313	C-103
5-Methyl-	3	0.570	184	69	BY-108

Table 1a. Alkanes (Page 3 of 3)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
6-Methyl-	4	0.790	184	96	BY-108
2,5-Dimethyl-	9	2.500	198	283	BY-108
4,6-Dimethyl-	9	62.000	198	7014	C-103
2,6,10-Trimethyl-	16	59.000	212	6234	C-103
2,7,10-Trimethyl-	6	5.300	212	560	C-102
2,6,11-Trimethyl-	11	48.000	212	5072	C-103
2-Methyl-6-propyl	4	0.040	226	4	BY-104
2-Methyl-8-propyl	8	2.900	226	287	BY-108
5,6-Diethyl-	2	0.076	226	8	BY-107
Tridecane	174	508.000	184	61843	C-103
2-Methyl-	22	21.000	198	2376	C-103
3-Methyl-	10	12.000	198	1358	C-103
4-Methyl-	13	1.500	198	170	BY-108
5-Methyl-	4	12.000	198	1358	C-103
6-Methyl-	14	29.000	198	3281	C-103
7-Methyl-	16	12.000	198	1358	BY-108
4,8-Dimethyl-	9	2.200	212	232	BY-108
3-Ethyl-	3	1.100	212	116	BY-107
5-Propyl-	4	1.900	226	188	BY-107
Tetradecane	134	121.000	198	13689	C-103
3-Methyl-	5	0.380	212	40	BY-108
4-Methyl-	4	3.100	212	328	BX-104
4-Ethyl-	1	0.040	226	4	BY-104
4,11-Dimethyl-	3	0.010	226	1	BY-105
2,6,10-Trimethyl-	4	0.190	240	18	BY-107
Pentadecane	48	37.000	212	3909	C-103
2-Methyl-	6	0.330	226	33	C-102
3-Methyl-	1	0.064	226	6	C-110
2,6,10-Trimethyl-	5	0.094	254	8	BY-107
2,6,10,14-Tetramethyl-	5	0.057	268	5	BY-107
8-Hexyl-	2	0.072	296	5	BY-107
Hexadecane	29	34.000	226	3370	C-103
2-Methyl-	2	0.067	240	6	BY-107
3-Methyl-	2	0.440	240	41	BY-107
7,9-Dimethyl-	3	0.012	254	1	B-103
2,6,10,14-Tetramethyl-	9	0.310	282	25	BY-110
Heptadecane	20	44.000	240	4107	C-103
3-Methyl-	1	0.051	254	4	C-110
7-Methyl-	1	0.500	254	44	BY-108
2,6,10,14-Tetramethyl-	1	0.046	296	3	BY-107
9-Octyl-	1	0.270	352	17	TY-103
Octadecane	8	0.074	254	7	BY-108
2-Methyl-	2	0.910	268	76	TY-103
Nonadecane	3	0.003	268	0.3	C-107
9-Methyl-	2	0.012	282	1	B-103
Eicosane	6	0.210	296	16	BY-107
Docosane					
7-Hexyl-	1	0.061	394	3	C-110
Hexacosane	1	0.030	366	2	BY-108
Total	**2731**	**1915.2**		**249,865**	

Table 1b. Alkanes Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Hexane						
3,4-Dimethyl-	1	0.005	114	1	C-107	583-48-2M
2,2,3-Trimethyl-	1	0.019	128	3	U-107	16747-25-4
2,2,4-Trimethyl-	1	0.012	128	2	TY-104	16747-26-5
2,3,3-Trimethyl-	1	0.002	128	0.4	T-107	16747-28-7
Heptane						
3,3-Dimethyl-	1	0.019	128	3	C-110	4032-86-4
4-Propyl-	1	0.010	142	1	A-102	3178-29-8
Octane						
2-Methyl-	1	0.020	128	4	BY-106	3221-61-2
3,4-Dimethyl-	1	0.009	142	1	BY-105	15869-92-8
3-Ethyl-2,7-dimethyl-	1	0.014	170	2	U-107	62183-55-5
Nonane						
5-Propyl-	1	0.004	170	1	C-104	998-35-6
2-Methyl-5-propyl-	1	0.002	184	0.2	T-107	31081-17-1
2,2,4,4,6,8,8-Heptamethyl-	1	0.013	226	1	S-105	4390-04-9
Decane						
2,4-Dimethyl-	1	0.003	170	0.4	BY-106	2801-84-5
5-Ethyl-5-methyl-	1	0.010	184	1	TX-118	17312-74-2
2,2,3-Trimethyl-	1	0.014	184	2	AX-102	62338-09-4
Undecane						
3-Ethyl-	1	0.002	184	0.3	TY-104	17312-58-2
6-Ethyl-	1	0.003	184	0.4	BY-106	17312-60-6
2,2-Dimethyl-	1	0.016	184	2	U-107	17312-64-0
3,5-Dimethyl-	1	0.001	184	0.1	C-112	17312-81-1
Dodecane						
2,2,4,9,11,11-Hexamethyl-	1	0.016	254	1	S-105	6304-50-3
Tridecane						
2,5-Dimethyl-	1	0.009	212	1	BY-103	56292-66-1
Tetradecane						
5-Methyl-	1	0.002	212	0.2	T-107	25117-32-2
2,5-Dimethyl-	1	0.010	226	1	BY-103	56292-69-4
6,9-Dimethyl-	1	0.001	226	0.1	T-107	55045-13-1
Heptadecane						
8-Methyl-	1	0.002	254	0.2	C-107	13287-23-5
2,6,10,15-Tetramethyl-	1	0.008	296	1	C-107	54833-48-6
Octadecane						
2,6-Dimethyl-	1	0.002	282	0.2	T-107	75163-97-2
Heneicosane	1	0.013	296	1	C-107	629-94-7
Total	**28**	**0.240**		**32**		

Table 2a. Cycloalkanes (Page 1 of 2)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
CYCLOALKANES						
Cyclopropane		38	0.380	42	203	BY-107
Methyl-		1	0.170	56	68	C-104
Ethyl-		5	7.300	70	2336	BY-108
1,1-Dimethyl-		4	0.510	70	163	BY-107
trans-1,2-Dimethyl-		1	0.049	70	16	BY-110
Propyl-		6	0.650	84	173	C-102
(1-Methylethyl)-		3	0.290	84	77	BY-104
Butyl		5	2.500	98	571	BY-108
(1-Methylbutyl)-		1	0.029	112	6	BY-110
Pentyl-		3	0.060	112	12	BY-109
Octyl-		2	1.200	154	175	C-102
1,2-Dibutyl-	(*)	1	0.042	154	6	BY-110
1-Pentyl-2-propyl-	(*)	1	1.600	154	233	C-101
1-Ethyl-2-heptyl-	(*)	1	0.060	168	8	BY-104
Cyclobutane		3	0.045	56	18	BY-107
Methyl-		1	1.400	70	448	U-103
Ethyl-		1	0.570	84	152	BY-107
(1-Methylethyl)-		3	0.160	98	37	BY-109
cis-1,2-Diethyl-	(**)	2	0.320	112	64	C-102
trans-1,2-Diethyl-		2	0.460	112	92	C-101
Cyclopentane		5	0.650	70	208	BY-107
Methyl-		12	2.100	84	560	BY-108
Ethyl-		3	0.040	98	9	BY-104
cis-1,2-Dimethyl-	(**)	5	0.340	98	78	S-103
trans-1,2-Dimethyl-		8	0.490	98	112	BY-108
cis-1,2-Dimethyl-trans-3-methyl-		3	0.032	112	6	BY-107
1,1,3-Trimethyl-	(*)	2	0.360	112	72	BY-108
1,2,4-Trimethyl-	(*)	1	0.180	112	36	S-103
a,a,b-1,2,4-Trimethyl-		4	0.030	112	6	BY-104
(1-Methylbutyl)-		2	0.240	140	38	BY-107
(2-Methylbutyl)-		2	0.350	140	56	BY-108
1,2-Dimethyl-3-(1-methylethyl)-	(*)	2	0.320	140	51	BY-107
1,3-Dimethyl-2-(1-methylethyl)-	(*)	5	0.760	140	122	BY-108
1-Methyl-3-(2-methylpropyl)-	(*)	5	0.570	140	91	BY-108
1-Butyl-2-ethyl-	(*)	2	0.110	154	16	BY-107
1-Butyl-2-propyl-	(*)	1	0.160	168	21	BY-107
1-Hexyl-3-methyl-	(*)	6	0.270	168	36	C-110
1-Pentyl-2-propyl-	(*)	4	0.470	182	58	C-102
Decyl		1	0.530	210	57	C-103
Cyclohexane		54	4.300	84	1147	C-103
Methyl-		41	1.600	98	366	TY-110
Ethyl-		5	0.460	112	92	BY-108
1,2-Dimethyl-	(*)	1	0.250	112	50	BY-108
cis-1,3-Dimethyl-		4	0.340	112	68	C-204
1,4-Dimethyl-	(*)	2	0.280	112	56	C-204
Cyclopropyl-		3	0.280	124	51	BY-108
Propyl-		3	0.110	126	20	C-102
1,1,2-Trimethyl-	(*)	2	1.500	126	267	C-204
1,1,3-Trimethyl-	(*)	10	0.810	126	144	BY-108
1,2,3-Trimethyl-	(*)	2	0.003	126	1	T-107
1,3,5-Trimethyl-	(*)	2	0.009	126	2	BY-106
Butyl-		6	1.500	140	240	BY-108
(1-Methylpropyl)-		5	2.100	140	336	C-103
cis-1-Ethyl-4-methyl-		6	0.570	140	91	BX-104
trans-1-Ethyl-4-methyl-		5	0.170	140	27	BY-108
1-Methyl-2-propyl-	(*)	2	0.078	140	12	T-111
1-Methyl-3-propyl-	(*)	4	0.590	140	94	C-102
1-Methyl-3-(1-methylethyl)-	(*)	1	0.340	140	54	C-110
cis-1-Methyl-4-(1-methylethyl)-		3	0.350	140	56	BY-108
1,1,2,3-Tetramethyl-	(*)	10	0.400	140	64	C-204
cis-1,1,3,5-Tetramethyl-		3	0.460	140	74	BX-104
trans-1,1,3,5-Tetramethyl-		2	0.021	140	3	C-110
1,1,4,4-Tetramethyl-	(*)	1	0.410	140	66	BY-108
a,a,a,a-1,2,4,5-Tetramethyl-		1	0.051	140	8	C-110
(1,2-Dimethylpropyl)-		1	0.170	154	25	BY-107
Pentyl-		21	2.400	154	349	C-204
1-Ethyl-2-propyl-	(*)	3	0.430	154	63	BY-108
1,1-Dimethyl-2-propyl-	(*)	5	0.300	154	44	C-102

Table 2a. Cycloalkanes (Page 2 of 2)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
1-Ethyl-2,2,6-trimethyl-	(*)	2	0.550	154	80	BY-108
(3-Methylpentyl)-		1	0.650	168	87	C-102
(4-Methylpentyl)-		5	2.700	168	360	BY-108
Hexyl-		14	0.670	168	89	BY-107
1-Methyl-2-pentyl-	(*)	3	0.530	168	71	BY-108
1-Methyl-2-pentyl-	(*)	3	0.530	168	71	BY-108
1-Methyl-3-pentyl-	(*)	3	0.077	168	10	C-110
1-Methyl-4-(1-methylbutyl)-	(*)	4	0.130	168	17	BY-107
1,2-Diethyl-1-methyl-	(*)	4	0.360	168	48	BY-108
1,2-Diethyl-3-methyl-	(*)	4	0.470	168	63	BY-108
2,4-Diethyl-1-methyl-	(*)	4	0.280	168	37	BY-107
1,5-Diethyl-2,3-dimehtyl-	(*)	2	0.570	168	76	C-102
(2,2-Dimethylcyclopentyl)-		4	0.310	180	39	BX-104
2-Butyl-1,1,3-trimethyl-	(*)	18	3.400	182	418	C-102
Octyl-		6	0.130	206	14	B-103
(1-Methylheptyl)-	(***)	1	2.600	206	283	BY-108
1,1,3-Trimethyl-2-(3-methylpentyl	(*)	5	0.740	210	79	BX-104
cis-(1-Cyclohexylmethyl)-2-methyl-		1	0.110	232	11	BY-107
trans-(1-Cyclohexylmethyl)-2-methyl-		1	0.250	232	24	BY-108
cis-(1-Cyclohexylmethyl)-4-methyl-		1	0.800	232	77	BY-108
(2-Ethyloctyl)-	(***)	3	0.048	234	5	BY-104
cis-(1-Cyclohexylmethyl)-2-ethyl-		3	1.000	246	91	BY-108
1,3,5,-Trimethyl-2-octadecyl-	(*)	2	0.140	378	8	BY-104
Cyclooctane						
Butyl-		1	0.330	168	44	C-102
cis-1,4-Dimethyl-		1	0.040	140	6	BY-104
Cycloundecane						
1,1,2-Trimethyl-	(*)	1	0.042	196	5	BY-109
Cyclododecane		7	2.700	168	360	C-102
Ethyl-		1	0.027	206	3	TY-103
Cyclhexadecane		4	0.100	224	10	S-110
DECALINS						
trans-Decahydronaphthalene		18	4.700	138	763	C-103
2-Methyl-	(*)	17	21.000	152	3095	C-103
1,2-Dimethyl-	(*)	1	1.400	168	187	C-102
1,5-Dimethyl-	(*)	3	0.029	168	4	BY-110
1,6-Dimethyl-	(*)	5	0.360	168	48	BY-108
2,3-Dimethyl-	(*)	7	3.100	168	413	C-204
2,6-Dimethyl-	(*)	8	2.500	168	333	C-204
2-Butyl-	(*)	1	0.320	180	40	BY-108
INDANES						
cis-Octahydro-1H-Indene		1	0.037	124	7	BY-110
trans-Octahydro-1H-indene						
2,2,4,4,7,7-Hexamethyl-		1	0.200	208	22	BY-107
OTHER BICYCLIC AND TRICYCLIC MOLECULES						
1,1'-Bicyclohexyl		1	0.046	168	6	BY-107
cis-2-Methyl-		1	0.120	182	15	BX-104
Bicyclo[2.2.1]heptane		3	0.020	96	5	BY-107
Bicyclo[4.1.0]heptane						
2-Methyl-7-pentyl-	(*)	1	1.300	180	162	C-204
3-Methyl-7-pentyl-	(*)	1	0.410	180	51	BY-108
Bicyclo[2.2.2]octane						
1,2,3,6-Tetramethyl-	(*)	1	0.060	166	8	C-110
Bicyclo[3.3.1]nonane		1	0.047	124	8	T-111
Total		**545**	**102.0**		**18,010**	

Notes
(*) The positional, geometrical or stereo isomer has not been defined.
(**) The concentration of the compound has been estimated from results for a mixture of isomeric compounds.
(***) The name used in this table differs from the name used in the data base.

Table 2b. Cycloalkanes Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
CYCLOALKANES							
Cyclopropane							
cis-1,2-Dimethyl-		1	0.0170	70	5	C-107	930-18-7
trans-1-Butyl-2-methyl-		1	0.0110	112	2	B-103	38851-70-6
1-Ethyl-2-pentyl-	(*)	1	0.0013	140	0.2	T-107	62238-08-8
1,1,2- Trimethyl-3-(2-methylpropyl)-		1	0.0100	140	2	BY-105	41977-43-9
1-Heptyl-2-methyl-	(*)	1	0.0150	154	2	BY-106	74663-91-5
1-Butyl-1-methyl-2-propyl-		1	0.0055	154	1	BY-105	41977-34-8
1-(2-Butyl)-1-(2-methylbutyl)-	(*)	1	0.0065	168	1	TY-104	UCY012-08
Cyclobutane							
1,1,2,3,3-Pentamethyl-		1	0.0080	126	1	C-108	57905-86-9
Cyclopentane							
cis-1,3-Dimethyl-		1	0.0060	98	1	BY-106	2532-58-3
cis-1-Ethyl-3-methyl-		1	0.0006	112	0.1	TY-104	2613-66-3
1,2,3- Trimethyl-	(*)	1	0.0048	112	1	AX-102	2815-57-8
(2-Methylpropyl)-		1	0.0250	126	4	TY-118	3788-32-7
2-Ethyl-1,1-dimethyl-		1	0.0022	126	0.4	SX-106	54549-80-3
cis-1,1,3,4- Tetramethyl-		1	0.0200	126	4	BY-104	53907-60-1
trans-1-Methyl-2-(4-methylpentyl)-		1	0.0006	168	0.1	TY-104	66553-50-2
3-Hexyl-1,1-dimethyl-		1	0.0035	182	0.4	TY-104	61142-65-2
Cyclohexane							
1,1-Dimethyl-		1	0.0047	112	1	TX-118	590-66-9
(1-Methylethyl)-		1	0.0070	126	1	BY-106	696-29-7
cis-1-Ethyl-2-methyl-		1	0.0160	126	3	BY-106	4923-77-7
a,b,b-1,2,4-Trimethyl-		1	0.0140	126	2	T-111	7667-60-9
(2-Methylpropyl)-		1	0.0092	140	1	A-102	1678-98-4
1-Methyl-4-(1-methylethyl)-	(*)	1	0.0230	140	4	T-111	99-82-1
1,2,4,5-Tetramethyl-	(*)	1	0.0100	140	2	BY-105	2090-38-2
1,2-Diethyl-1-methyl-		1	0.0050	154	1	BY-106	61141-79-5
(1,2-Dimethylbutyl)-		1	0.0083	168	1	B-103	61142-37-8
2-Propyl-1,1,3-trimetnyl-	(*)	1	0.0060	168	1	BY-106	UCY012-04
1,2-Dimethyl-3-pentyl-		1	0.0093	182	1	B-112	UCY013-03
trans-1-(Cyclohexylmethyl)-4-methyl-		1	0.0100	196	1	BY-105	54823-98-2
cis-1-(Cyclohexylmethyl)-4-ethyl-		1	0.0047	210	1	C-109	54934-95-1
(1-Propylheptyl)-		1	0.0020	224	0.2	C-111	13151-75-2
Decyl-		1	0.0020	224	0.2	BY-105	1795-16-0
Cyclooctane		1	0.0060	112	1	TY-104	292-64-8
1,5-Dimethyl-	(*)	1	0.0100	140	2	BY-105	21328-57-4
Cyclotetradecane		1	0.0270	196	3	T-111	295-17-0M
OTHER BICYCLIC AND TRICYCLIC MOLECULES							
1,1'-Bicyclohexyl							
trans-2-methyl-		1	0.0220	180	3	C-110	50991-09-8
Bicyclo[4.1.0]heptane		1	0.0230	96	5	C-110	286-08-8
Total		**36**	**0.3562**		**60**		

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 3a. Alkenes and Alkadienes (Page 1 of 3)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALKENES						
Propene		42	8.300	42	4427	BY-108
2-Methyl-		70	16.000	56	6400	C-103
1-Butene		28	23.000	56	9200	C-103
2-Methyl-		4	0.210	70	67	BY-108
3-Methyl-		4	1.500	70	480	BY-108
2,3-Dimethyl-		1	0.025	84	7	BY-105
3,3-Dimethyl-		1	0.032	84	9	U-106
2-Butene						
2-Methyl-		3	0.160	70	51	BY-104
2,3-Dimethyl-		1	0.130	84	35	BY-104
E-2-Butene	(*)	5	0.130	56	52	C-104
Z-2-Butene	(*)	5	1.600	56	640	C-103
1-Pentene		18	10.000	70	3200	C-103
2-Methyl-		6	2.600	84	693	BY-108
4-Methyl-		14	2.500	84	667	BY-108
3,4-Dimethyl-		2	1.800	98	411	BY-108
4,4-Dimethyl-		2	0.050	98	11	TX-111
2-Pentene						
2,4-Dimethyl-		2	0.037	98	8	B-103
E-2-Pentene	(*)	4	0.950	70	304	BY-107
4-Methyl-		1	0.028	84	7	BY-106
Z-2-Pentene	(*)	11	1.300	70	416	BY-108
1-Hexene		49	13.000	84	3467	C-103
4-Methyl-		1	0.440	98	101	S-103
5-Methyl-		3	1.600	98	366	BY-108
4-Ethyl-		1	0.210	112	42	S-103
3,4-Dimethyl-		4	0.340	112	68	BY-107
4,5-Dimethyl-		3	0.340	112	68	BY-108
5,5-Dimethyl-		2	0.018	112	4	C-110
3,4,5-Trimethyl-		1	0.039	126	7	TX-111
E-2-Hexene		1	0.088	84	23	BY-104
Z-2-Hexene		2	0.040	84	11	BY-105
4,4,5-Trimethyl-		1	0.034	126	6	U-106
Z-3-Hexene						
2,3,4,5-Tetramethyl-		2	0.079	140	13	C-110
3-Ethyl-2,5-dimethyl-	(**)	2	0.280	140	45	BY-107
1-Heptene		17	1.700	98	389	BY-108
3-Methyl-		2	0.780	112	156	BY-108
5-Methyl-		2	0.110	112	22	BY-109
6-Methyl-		2	0.740	112	148	BY-107
2,4-Dimethyl-		1	0.120	126	21	BX-102
E-2-Heptene		7	0.032	98	7	B-103
Z-2-Heptene		3	0.040	98	9	BY-105
3-Methyl-	(*)	1	0.700	112	140	TX-116
E-3-Heptene	(*)	2	0.023	98	5	BY-104
Z-3-Heptene		1	0.026	98	6	B-103
2,2,3,5,5,6,6-Heptamethyl-		2	0.220	196	25	C-101
1-Octene		7	0.920	112	184	BY-108
3-Ethyl-		1	0.190	140	30	S-103
2-Octene	(**)	1	0.680	112	136	TX-116
E-3-Octene	(*)	2	0.130	112	26	BY-104
Z-3-Octene	(*)	1	0.390	112	78	BY-108
1-Nonene		1	0.460	126	82	BY-108
4-Nonene						
5-Butyl-		5	0.140	182	17	TY-103
Z-4-Nonene						
2,3,3-Trimethyl-		3	0.570	168	76	BY-108
1-Decene		5	0.044	140	7	U-103
E-2-Decene		1	0.043	140	7	C-102
Z-2-Decene						
4-Methyl-		2	0.660	154	96	C-102
3-Decene	(**)	2	0.150	140	24	C-101
E-4-Decene						

Table 3a. Alkenes and Alkadienes (Page 2 of 3)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
3-Methyl-		1	0.190	154	28	BY-107
5-Decene		1	0.740	140	118	BY-108
E-5-Decene		2	0.023	140	4	B-103
1-Undecene		4	0.320	154	47	BY-108
4-Methyl-		3	1.500	168	200	BY-108
7-Methyl-		2	0.080	168	11	C-110
8-Methyl-		1	0.050	168	7	C-110
E-2-Undecene						
6-Methyl-		1	0.180	168	24	BY-107
7-Methyl-		1	0.082	168	11	BY-107
2,5-Dimethyl-		1	0.091	182	11	U-106
Z-2-Undecene						
8-Methyl-	(**)	1	0.380	168	51	BY-108
2,5-Dimethyl-		1	0.091	182	11	BY-107
E-3-Undecene		2	0.023	154	3	T-111
Z-3-Undecene	(**)					
2-Methyl-		2	3.300	168	440	C-102
4-Undecene						
4-Methyl-	(**)	2	2.000	168	267	C-102
6-Methyl-	(**)	2	0.240	168	32	BX-104
Z-4-Undecene						
5-Methyl-		1	0.270	168	36	C-102
E-5-Undecene	(*)	6	1.500	154	218	BY-108
7-Methyl-	(*)	1	0.740	168	99	C-102
Z-5-Undecene		6	1.500	154	218	BY-108
7-Methyl-		1	0.110	168	15	BY-107
1-Dodecene		6	0.430	168	57	C-102
E-3-Dodecene		4	0.170	168	23	TY-103
Z-3-Dodecene		1	0.300	168	40	BY-108
E-4-Dodecene		3	0.610	168	81	C-102
1-Tridecene		7	0.100	182	12	C-110
6-Tridecene	(**)	3	0.110	182	14	TY-103
7-Methyl-	(**)	5	2.300	196	263	BY-108
1-Tetradecene		4	5.700	196	651	C-103
E-3-Tetradecene		3	0.710	196	81	BY-107
Z-3-Tetradecene		1	0.250	196	29	C-110
E-5-Tetradecene		2	0.630	196	72	BY-108
Z-6-Tetradecene		2	0.040	196	5	BY-105
Z-7-Tetradecene	(*)	4	0.019	196	2	T-111
1-Pentadecene		4	0.330	210	35	BY-107
1-Hexadecene		6	2.600	224	260	C-103
Z-3-Hexadecene		2	0.040	224	4	BY-104
Z-7-Hexadecene		3	0.220	224	22	BY-108
E-5-Eicosene		1	0.680	294	52	BY-108
ALKADIENES						
1,3-Butadiene		17	0.560	54	232	C-204
2-Methyl-		3	0.160	68	53	BY-104
2,3-Dimethyl-		1	0.048	82	13	BY-106
1,2-Pentadiene		1	0.033	68	11	BY-105
E-1,3-Pentadiene		1	0.027	68	9	BY-106
Z-1,3-Pentadiene		1	0.084	68	28	BY-110
2-Methyl-	(*)	4	1.500	82	410	BY-108
1,4-Hexadiene	(**)	5	0.160	82	44	BY-104
4-Methyl-	(**)	2	0.030	96	7	BY-104
1,5-Hexadiene		1	0.120	68	40	BY-104
2,6-Octadiene	(**)					
4,5-Dimethyl-	(**)	1	0.028	138	5	BY-109
3,4-Nonadiene		1	0.480	124	87	BY-108
4,5-Nonadiene		1	0.600	124	108	C-102
E,E-4,6-Decadiene						
3,8-Dimethyl-		1	0.470	166	63	BY-106
POLYENES						

Table 3a. Alkenes and Alkadienes (Page 3 of 3)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
2,6,10,14,18,22-Tetracosahexaene					
2,6,10,19,23-Pentamethyl-	2	1.100	406	61	BY-109
2,6,10,15,19,23-Hexamethyl-	1	1.200	420	64	BY-109
Total	**513**	**131.0**		**37782**	

Notes
(*) The observations for unresolved mixtures have been included.
(**) The positional, geometrical or stereo isomer has not been defined.

Table 3b. Alkenes and Alkadienes Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
ALKENES							
1-Butene							
2,3-Dimethyl-		1	0.0250	84	7	BY-105	563-78-0
1-Pentene							
2,2,4-Trimethyl-		1	0.0190	112	4	T-111	107-39-1
2-Pentene							
3-Ethyl-		1	0.0100	98	2	TY-104	816-79-5
1-Hexene							
2-Methyl-		1	0.0040	98	1	BY-106	6094-02-6
3,5,5-Trimethyl-		1	0.0100	126	2	BY-105	4316-65-8
2-Hexene							
2,4-Dimethyl-		1	0.0090	112	2	C-105	14255-23-3
3-Heptene							
4-Propyl-	(*)	1	0.0130	140	2	B-103	4485-13-6
1-Octene							
7-Methyl-		1	0.0220	126	4	C-104	13151-06-9
E-4-Octene		1	0.0100	112	2	BY-105	14850-23-8
E-2-Nonene		1	0.0007	126	0.1	TY-104	6434-78-2
4-Nonene							
5-Methyl-		1	0.0030	140	0.5	BY-106	15918-07-7
1-Decene							
4-Methyl-		1	0.0080	154	1	TY-104	13151-29-6
5-Methyl-		1	0.0019	154	0.3	TY-104	54244-79-0
3,4-Dimethyl-		1	0.0130	168	2	TY-104	
4-Decene							
7-Methyl-		1	0.0070	154	1	TY-104	UAE011-05
2-Undecene							
4-Methyl-	(*)	1	0.0035	168	0.5	TY-104	91695-32-8
E-2-Undecene							
4,5-Dimethyl-		1	0.0011	182	0.1	U-106	55170-92-8
Z-2-Undecene		1	0.0006	154	0.1	TY-104	821-96-5
3-Undecene							
5-Methyl-	(*)	1	0.0080	168	1	TY-104	UAE012-06
8-Methyl-	(*)	1	0.0100	168	1	BY-105	UAE012-04
E-4-Undecene		1	0.0040	154	1	C-107	693-62-9
2-Dodecene							
4-Methyl-	(*)	1	0.0022	182	0.3	C-110	56851-45-7
Z-5-Dodecene		1	0.0073	168	1	BY-106	7206-28-2
E-6-Dodecene		1	0.0100	168	1	BY-105	7206-17-9
1-Heptadecene		1	0.0078	238	1	SX-103	6765-39-5
1-Octadecene		1	0.0020	252	0.2	C-111	112-88-9
1-Nonadecene		1	0.0010	266	0.1	C-109	18435-45-5
ALKADIENES							
1,3-Pentadiene							
2,3-Dimethyl-		1	0.0110	96	3	TY-104	1113-56-0
1,4-Pentadiene							
2,3-Dimethyl-		1	0.0075	96	2	SX-106	758-86-1
Z-1,3-Hexadiene							
3-Ethyl-2-methyl-		1	0.0052	124	1	AX-101	74752-97-9
1,4-Hexadiene							
2,3-Dimethyl-	(*)	1	0.0050	110	1	AX-101	18669-52-8
1,11-Dodecadiene		1	0.0040	166	1	TY-104	5876-87-9
1,12-Tridecadiene		1	0.0050	180	1	C-105	21964-48-7
Total		**33**	**0.2508**		**45**		

NOTES
(*) The positional, geometrical or stereo isomer has not been defined.

Table 4a. Alkynes

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
Propyne	4	0.610	40	342	C-102
4-Nonyne	1	0.610	124	110	BY-108
3-Decyne	2	0.510	138	83	BY-108
3-Hexadecyne	1	0.500	222	50	C-102
Total	**8**	**2.230**		**585**	

Table 4b. Alkynes Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
1-Nonyne	1	0.010	124	2	BY-105	3452-09-3
1-Octadecyne	1	0.002	252	0.2	T-107	629-89-0
Total	**2**	**0.012**		**2**		

Table 5a. Benzene, Biphenyl, Napthalene, Fluorene and Their Alkyl and Alkenyl Derivatives

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
BENZENE AND ALKYLBENZENES					
Benzene	175	7.500	78	2154	BY-104
Monosubstituted Benzenes					
Methyl-	208	4.800	92	1169	BX-103
Ethyl-	110	0.660	106	139	BX-103
(1-Methylethyl)-	2	0.470	120	88	C-102
Propyl-	4	0.028	120	5	C-110
(1,1-Dimethylethyl)-	2	0.053	134	9	C-110
Pentyl-	2	1.400	148	212	C-102
(1-Methylpentyl)-	1	0.890	162	123	C-102
(1-Methylhexyl)-	1	0.720	176	92	C-102
(1-Methylheptyl)-	1	0.180	190	21	C-102
(1-Methyldecyl)-	2	0.006	232	1	C-104
(1-Propylnonyl)-	2	0.005	246	0.5	C-104
(1-Butylheptyl)-	2	0.005	232	0.5	C-104
(1-Pentylheptyl)-	2	0.007	246	1	C-104
Disubstituted Benzenes					
1,2-Dimethyl-	98	0.780	106	165	BY-108
1,3- and 1,4-Dimethyl-	128	1.800	106	380	BX-103
1-Ethyl-2-methyl-	40	0.044	120	8	C-110
1-Ethyl-3-methyl-	1	0.036	120	7	SX-107
1-Ethyl-3-methyl-	4	0.011	120	2	BY-104
1-Methyl-2-propyl-	1	0.870	134	145	C-102
Trisubstituted Benzenes					
1,2,4-Trimethyl-	63	0.078	120	15	C-107
1,3,5-Trimethyl-	48	0.052	120	10	U-112
BIPHENYL					
1,1'-Biphenyl	6	15.000	154	2182	C-103
2-Methyl-	3	1.800	168	240	C-102
2,2'-Diethyl-	4	0.003	210	0.3	TX-105
OTHER ARENES					
Naphthalene	8	0.045	128	8	SX-112
2-Methyl-	1	0.027	142	4	T-111
(9H)Fluorene	2	0.017	166	2	C-102
ALKENYLBENZENES					
Benzene					
1-Ethenyl-	48	1.300	104	280	C-103
(1-Methylethenyl)-	2	0.014	118	3	C-108
(1-Propenyl)- (*)	2	0.630	118	120	C-102
(2-Propenyl)-	2	0.290	118	55	C-101
(2-Methyl-2-propenyl)-	1	0.590	132	100	C-102
Total	**976**	**40.111**		**7740**	

Notes
(*) The positional, geometrical or stereo isomer has not been defined.

Table 5b. Benzene, Biphenyl, Napthalene, Fluorene and Their Alkyl and Alkenyl Derivatives Observed in One Tank at Concentrations Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Monosubstituted Benzenes						
(1-Methylpropyl)-	1	0.0200	134	3	T-111	135-98-8
(1,1-Dimethylpropyl)-	1	0.0190	148	3	T-111	2049-95-8
(1-Ethylnonyl)-	1	0.0080	218	1	C-105	4536-87-2
(1-Butyloctyl)-	1	0.0060	246	1	C-105	2719-63-3
(1-Methylundecyl)-	1	0.0050	246	0.5	C-104	2719-61-1
Disubstituted Benzenes						
1-Methyl-3-(1-methylethyl)-	1	0.0140	134	2	T-111	535-77-3
1-Isopropyl-2-methyl-	1	0.0200	134	3	SX-107	527-84-4
Trisubstituted Benzenes						
1,2,3-Trimethyl-	1	0.0240	120	4	SX-107	526-73-8
bis-1,1'-(1,4-Butanediyl)benzene	1	0.0130	210	1	TX-105	1083-56-3
Naphthalene						
1-Methyl-	1	0.0240	142	4	SX-107	90-12-0
1,7-Dimethyl-	1	0.0110	156	2	T-111	575-37-1
2,3-Dimethyl-	1	0.0120	156	2	T-111	581-40-8
Total	**12**	**0.1760**		**27**		

Table 6a. Halogen Containing Compounds (Page 1 of 1)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
HALO ALKANES					
Methane					
Chloro-	72	0.230	51	101	TX-110
Dichloro-	113	6.900	85	1818	BY-108
Chlorodifluoro-	9	6.500	87	1674	BX-111
Bromo-	12	0.059	95	14	U-112
Dichlorofluoro-	14	0.250	103	54	AX-102
Trichloro-	33	0.082	120	15	TX-105
Dichlorodifluoro-	74	0.110	121	20	SX-101
Trichlorofluoro-	257	180.000	138	29217	BY-104
Tetrachloro-	55	2.200	154	320	TX-105
Ethane					
Chloro-	29	0.113	65	39	C-107
1,1-Dichloro-	9	0.047	99	11	U-112
1,2-Dichloro-	8	0.055	99	12	U-112
1-Chloro-1,1-difluoro-	18	3.300	101	732	U-109
1,1-Dichloro-1-fluoro	15	0.940	117	180	S-101
1,1,1-Trichloro-	44	0.068	134	11	BY-108
1,1,2-Trichloro-	30	0.500	134	84	BY-108
1,1,2,2-Tetrachloro-	19	0.160	168	21	BY-108
1,2-Dichloro-1,1,2,2-tetrafluoro-	13	0.167	171	22	BY-108
1,1,2-Trichloro-1,2,2-trifluoro-	63	0.440	187	53	TY-108
1,2-Dibromo-	13	0.084	188	10	U-112
Propane					
1-Fluoro-	1	0.160	62	58	BY-110
1,2-Dichloro-	6	0.066	113	13	BY-108
Butane					
1-Chloro-	5	0.200	93	48	A-101
2-Bromo-	2	0.140	137	23	C-101
HALO ALKENES					
Ethene					
Fluoro-	2	0.410	46	200	C-109
Chloro-	9	0.030	63	11	U-112
1,1-Dichloro-	45	0.089	97	21	S-101
Z-1,2-Dichloro-	14	9.800	97	2263	U-112
Trichloro-	34	0.410	132	70	BY-108
Tetrachloro-	112	0.770	166	104	BY-107
Propene					
2-Fluoro-	5	1.400	60	523	BY-108
3-Chloro-	2	0.022	77	6	U-112
E-1,3-Dichloro-	8	10.000	111	2018	BY-108
Z-1,3-Dichloro-	6	9.200	111	1857	U-112
1,3-Butadiene					
Hexachloro-	17	10.000	261	858	BY-108
AROMATIC HALOGEN COMPOUNDS					
Benzene					
Chloro-	29	0.075	113	15	BY-108
1,2-Dichloro-	9	0.053	147	8	U-112
1,3-Dichloro-	18	0.066	147	10	BY-108
1,4-Dichloro-	23	0.021	147	3	B-107
1,2,4-Trichloro-	12	0.130	182	16	BY-110
1,1'-Biphenyl					
2-Chloro-	5	0.038	189	5	TY-103
3-Chloro-	2	0.036	189	4	B-103
2,2'-Dichloro-	2	0.006	223	1	BY-112
2,6-Dichloro-	2	0.004	223	0.4	TY-104
2,3,3',5'-Tetrachloro-	2	0.005	292	0.4	TY-105
2,3,4',6-Tetrachloro-	2	0.003	292	0.2	TY-103
OTHER					
1,1,1-Trifluoropropanone	1	0.052	112	10	U-103
1-Butanamine					
1,1,2,2,3,3,4,4,4-Nonafluoro-N,N-bis(nonafluorobutyl)-	1	0.083	671	3	C-109
Benzeneethanamine					
N-[Perfluorophenyl]-beta,4-bis[TMSoxy] (*)	1	0.082	462	4	U-112
Butanamide					
Perfluoro-N-[2-TMSoxy-2-[4-TMSoxy]phenyl]ethyl- (*)	1	0.180	488	8	U-106
Methane					
Fluorotrinitro-	1	0.110	169	15	BX-103
Total	**1278**	**245.7**		**42568**	

Note

(*) 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.

(**) The trimethylsilyl fragment is designated as TMS in this table.

Table 6b. Halogen Containing Compounds Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
HALOALKANES						
Propane						
1-Chloro-2,2-dimethyl-	1	0.0180	107	4	U-105	753-89-9
Octane						
2-Chloro-	1	0.0047	149	1	TX-118	628-61-5
AROMATIC HALOGEN COMPOUNDS						
Benzene						
1-Chloro-4-nitro-	1	0.0053	134	1	C-107	100-00-5
Biphenyl						
4-Chloro-	1	0.0028	189	0.3	TY-104	2051-62-9
2,3-Dichloro-	1	0.0011	223	0.1	TY-104	16605-91-7
2,5-Dichloro-	1	0.0010	223	0.1	TY-104	34883-39-1
3,3'-Dichloro-	1	0.0075	223	1	TX-118	2050-67-1
4,4'-Dichloro-	1	0.0041	223	0.4	TY-104	2050-68-2
2,2,4'-Trichloro-	1	0.0026	257	0.2	TY-104	7012-37-5
2,4',5-Trichloro-	1	0.0038	257	0.3	TY-104	16606-02-3
2,3,4-Trichloro-	1	0.0019	257	0.2	TY-104	55702-46-0
OTHER HALOGEN COMPOUNDS						
Silane						
Fluorotrimethyl-	1	0.0020	92	0.5	T-107	420-56-4
Total	**12**	**0.05480**		**8.279**		

Table 7a. Alcohols, Phenols, and Ethers (Page 1 of 2)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALKANOLS					
Methanol	155	30.000	32	21000	S-102
Ethanol	172	44.000	46	21426	S-102
2-Butoxy-	11	0.320	118	61	BY-104
2-Tetradecyloxy-	1	2.100	258	182	BY-108
1-Propanol	171	4.700	60	1755	BY-107
2-Methyl-	6	0.060	74	18	TY-104
2,2-Dimethyl-	7	7.800	88	1985	C-103
1-Cyclopentyl-2,2-dimethyl-	2	0.012	156	2	U-112
2-Propanol	65	5.300	60	1979	BY-108
1-(1-Methylethoxy)-	1	0.033	118	6	U-107
2-Methyl-	30	0.330	74	100	TX-110
2-Propyl-	77	5.300	102	1164	TX-110
1-Butanol	222	193.000	74	58422	BY-108
2-Methyl-	4	0.160	88	41	C-101
3-Methyl-	2	0.110	88	28	BX-104
2-Ethyl-	2	0.064	102	14	TY-103
3,3-Dimethyl-	3	0.083	102	18	TX-111
2-Butanol	24	0.680	74	206	BY-107
2-Methyl-	3	0.070	88	18	BY-104
1-Pentanol	17	0.190	88	48	BX-104
4-Methyl-2-propyl-	1	0.035	144	5	TY-103
2-Pentanol	3	0.550	88	140	BY-107
2-Methyl-	6	0.230	102	51	BY-107
2,3-Dimethyl-	2	0.006	116	1	BY-106
3-Ethyl-2-methyl-	2	0.001	130	0.2	T-107
3-Pentanol					
2-Methyl-	3	0.150	102	33	BY-108
1-Hexanol	16	0.210	102	46	BX-103
2-Ethyl-	44	1.600	130	276	C-103
3-Hexanol	1	0.037	102	8	U-106
2-Methyl-	1	0.093	116	18	BY-102
1-Heptanol	15	2.100	116	406	C-103
2-Heptanol	2	0.270	116	52	BY-107
2-Methyl-	2	0.003	130	1	BY-106
3-Heptanol	18	0.310	116	60	BY-107
1-Octanol	16	0.360	130	62	BY-108
2-Butyl-	5	0.350	186	42	BY-108
2-Octanol	4	0.410	130	71	BY-108
2-Methyl-	1	0.036	144	6	BY-102
1-Nonanol	9	0.024	144	4	BY-102
1-Decanol	2	0.002	158	0.3	C-109
1-Dodecanol	3	0.008	186	1	C-104
6-Dodecanol	2	0.014	186	2	B-103
1-Tetradecanol	2	0.010	214	1	BY-105
1-Hexadecanol	15	11.000	242	1018	C-204
1-Octadecanol	4	12.000	270	996	C-204
CYCLOALKANOLS					
Cyclopentanol	5	7.300	100	1635	C-103
ALKANDIOLS					
1,2-Propandiol	14	0.510	76	150	A-101
ALKENOLS, ALKENDIOLS, AND ALKYNEOLS					
2-Propen-1-ol	2	0.010	58	4	SX-106
Z-2-Buten-1-ol	2	0.120	72	37	C-101
3-Buten-1-ol	2	18.000	72	5600	BY-108
3-Buten-2-ol	7	4.800	72	1493	BY-108
1,4-Pentadien-3-ol	1	0.027	84	7	BY-110
5-Hexen-1-ol	1	0.071	100	16	AX-102
Z-3-Octen-2-ol					

Table 7a. Alcohols, Phenols, and Ethers (Page 2 of 2)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
2-Methyl-	2	0.370	142	58	C-101
1-Dodecyn-4-ol	1	0.042	182	5	BY-103
6,10-Dodecadien-1-ol					
3,7,11-Trimethyl-	1	2.600	224	260	C-103
ETHERS					
Dimethyl Ether	11	4.200	46	2045	C-103
Butane					
1-Methoxy-	1	0.044	88	11	TX-111
Dibutyl Ether	8	2.300	130	396	C-103
E-2-Pentene					
5-Pentyloxy-	2	0.024	156	3	C-104
Hexane					
3-Methoxy-	2	0.240	116	46	BY-107
1-Ethoxy-	1	0.110	130	19	TY-103
Cycloheptane					
Methoxy-	2	0.110	128	19	C-101
trans-1,3-Dimethoxy-	1	0.002	158	0.3	T-107
Didecyl ether	4	0.970	298	73	BY-108
Divinyl ether	1	0.097	70	31	C-107
Diphenyl Ether	2	0.180	170	24	T-111
PHENOLS					
Phenol	10	0.087	94	21	BY-107
2-Methyl-	3	0.040	108	8	BY-104
3-Methyl-	2	0.010	108	2	BY-105
Total	**1242**	**366.4**		**123,737**	

Table 7b. Alcohols, Phenols, and Ethers Observed in One Tank at Concentration Less Than 0.025 mg/m^3 (Page 1 of 2)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
ALKANOLS							
Methanol							
Dimethyl-(cyclooctyl)-		1	0.0180	170	2	T-111	16624-06-9
1-Pentanol							
5-Methoxy		1	0.0110	118	2	BY-106	4799-62-6
3-Pentanol							
2,3,4-Trimethyl-		1	0.0100	130	2	T-111	30544-92-0
2-Hexanol							
5-Methyl-		1	0.0027	116	1	T-107	627-59-8
2,3-Dimethyl-		1	0.0007	130	0.1	TY-104	19550-03-9
2-Heptanol							
3-Ethyl-2-methyl-		1	0.0069	158	1	BY-112	19780-59-7
3-Octanol							
6-Ethyl-		1	0.0089	158	1	B-103	19781-27-2
3,7-Dimethyl-		1	0.0088	158	1	T-111	57706-88-4
1-Decanol							
2-Ethyl-		1	0.0010	186	0.1	TY-104	21078-65-9
2-Decanol		1	0.0048	158	1	TY-104	1120-06-5
3-Decanol		1	0.0180	158	3	BY-103	1565-81-7
5-Decanol		1	0.0250	158	4	B-103	5205-34-5
1-Undecanol		1	0.0053	172	1	TX-118	112-42-5
2-Undecanol		1	0.0035	172	0.5	TY-104	1653-30-1
4-Undecanol		1	0.0023	172	0.3	T-107	4672-06-4
3-Dodecanol		1	0.0085	186	1	TY-104	10203-30-2
1-Tridecanol		1	0.0097	200	1	T-111	26248-42-0
2-Tridecanol		1	0.0050	200	1	C-105	1653-31-2
1-Pentadecanol		1	0.0210	228	2	TY-101	629-76-5
1-Hexadecanol							
2-Methyl-		1	0.0045	256	0.4	C-108	2490-48-4
1-Heptadecanol		1	0.0230	256	2	BY-110	1454-85-9
16-Methyl-		1	0.0040	270	0.3	C-111	41744-75-6
1-Nonadecanol		1	0.0090	284	1	S-105	1454-84-8
ALKENOLS AND ALKYNOLS							
1-Pentyne-3-ol							
3,4-Dimethyl-		1	0.0027	112	1	SX-106	1482-15-1
1-Tridecyne-4-ol		1	0.0057	196	1	C-110	74646-37-0
Z-9-Octadecene-1-ol		1	0.0050	268	0.4	C-111	143-28-2
DIOLS							
2,3-Butanediol							
2,3-Dimethyl- (Racemate or meso)		1	0.0090	118	2	BY-103	76-09-5
3-Hexyne-2,5-diol							
2,5-Dimethyl-		1	0.0023	142	0.4	TY-104	142-30-3
2,7-Octanediol							
2,7-Dimethyl-		1	0.0210	174	3	T-111	19781-07-8
1,12-Dodecanediol		1	0.0010	202	0.1	C-109	5675-51-4
CYCLIC ALCOHOLS							
Cyclohexanol		1	0.0022	100	0.5	S-111	108-93-0
4-(1,1,3,3-Tetramethylbutyl-)	(*)	1	0.0043	212	0.5	BY-106	4631-98-5
4-Methyl-1-(1-methylethyl)-		1	0.0013	156	0.2	TY-104	470-65-5
Cycloheptanol							
1-Methyl-		1	0.0010	128	0.2	TY-104	3761-94-2
Bicyclo[3.1.1]hept-3-en-2-ol							
4,6,6-Trimethyl-	(*)	1	0.0060	152	1	C-104	13040-03-4
ETHERS							
Ethane							
1,2-Dimethoxy-		1	0.0100	90	2	BY-105	110-71-4
Propane							
2-Ethoxy-2-methyl-		1	0.0011	102	0.2	TY-104	637-92-3
Butane							
Cycloheptane							
trans-1,3-Dimethoxy-		1	0.0020	142	0.3	T-107	29887-79-4
Benzene							
1-Butoxy-4-methoxy-		1	0.0040	180	0.5	C-105	20743-96-7
PHENOLS							
Phenol							
4-Propyl-		1	0.0031	136	1	SX-103	645-56-7
4-(1,1-Dimethylethyl)-		1	0.0013	136	0.2	C-109	98-54-4
2-(1,1-Dimethylethyl)-4-methoxy-		1	0.0040	150	1	TY-104	121-00-6

Table 7b. Alcohols, Phenols, and Ethers Observed in One Tank at Concentration Less Than 0.025 mg/m^3 (Page 2 of 2)

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
1,3-Benzenediol						
2-Methyl-	1	0.0055	124	1	C-107	608-25-3
4-Hexyl-	1	0.0055	194	1	C-105	136-77-6
Total	**43**	**0.3041**		**41**		

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 8a. Aldehydes

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALIPHATIC ALDEHYDES						
Ethanal		41	0.700	44	356	BX-104
Propanal		9	0.560	58	216	BX-103
2-Methyl-		2	0.011	72	3	S-110
2,2-Dimethyl-		2	0.030	86	8	B-103
Butanal		107	72.000	72	22400	C-102
2-Methyl-		3	0.080	86	21	BX-104
3-Methyl-		3	0.110	86	29	B-103
Pentanal		15	0.920	86	240	C-101
2-Methyl-		2	0.230	100	52	BY-104
3-Methyl-		2	0.190	100	43	U-107
Hexanal		41	5.700	100	1277	C-103
3-Methyl-		3	0.730	114	143	BY-108
2-Ethyl-		4	0.190	128	33	B-103
Heptanal		33	0.600	114	118	C-102
Octanal		28	2.600	128	455	C-103
Nonanal		31	6.600	142	1041	C-103
Decanal		17	0.031	156	4	BY-109
Undecanal		3	0.004	170	1	C-111
Dodecanal		3	0.006	184	1	C-111
ALKENALS						
Prop-2-enal		2	0.015	56	6	B-103
2-Methyl-		3	0.080	70	26	TY-104
E-But-2-enal		9	0.072	70	23	C-105
2-Methyl- Pent-4-enal		1	0.052	84	14	B-103
2-Ethyl-	(*)	1	0.070	112	14	BY-104
E-Hex-2-enal		4	0.310	98	71	C-101
Z-Hept-4-enal		2	0.010	112	2	BY-105
Hept-5-enal 2,6-Dimethyl-	(*)	1	0.420	140	67	BY-108
E-Non-2-enal		3	0.018	140	3	BY-110
Decadienal E,E-Dodeca-7,9-dienal		1	0.054	180	7	C-204
Octadec-2-enal	(*)	2	0.024	266	2	BY-103
AROMATIC ALDEHYDES						
Benzaldehyde		4	0.032	106	7	U-106
Total		**382**	**92.4**		**26,681**	

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 8b. Aldehydes Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
ALKANALS							
Octanal							
7-Hydroxy-3,7-dimethyl-		1	0.001	156	0.1	T-107	107-75-5
Tridecanal		1	0.002	198	0.2	C-107	10486-19-8
Hexadecanal		1	0.0047	240	0.4	BY-111	629-80-1
ALKENALS							
Z-3-Hexenal		1	0.021	98	5	U-103	6789-80-6
E-2-Octeneal		1	0.009	112	2	AX-101	2548-87-0
E,E-2,4-Nonadienal		1	0.0054	124	1	AX-101	5910-87-2
E-2-Deceneal		1	0.0043	154	1	AX-101	3913-81-3
2-Dodeceneal	(*)	1	0.004	182	0.5	C-109	4826-62-4
CYCLIC COMPOUNDS							
Cyclohexanal							
4-(1-methylethyl)-	(*)	1	0.021	154	3	C-110	UAD010-02
Cyclohex-3-en-1-al							
1,3,4-Trimethyl-	(*)	1	0.005	152	1	TY-104	40702-26-9
BENZENE DERIVATIVES							
Benzaldehyde							
3-Phenoxy-		1	0.002	182	0.2	C-107	39515-51-0
Total		**11**	**0.079**		**14**		

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 9a. Ketones (Page 1 of 2)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALIPHATIC KETONES						
2-Propanone		261	50.000	58	19310	C-103
2-Butanone		192	42.000	72	13067	C-103
3-Methyl-		19	7.100	86	1849	C-103
3,3-Dimethyl-		17	0.110	100	25	TX-110
2-Pentanone		80	4.500	86	1172	C-103
3-Methyl-		6	0.160	100	36	BY-107
4-Methyl-		88	4.200	100	941	C-103
4,4-Dimethyl-		14	0.140	114	28	BY-112
3-Pentanone		4	0.042	86	11	BY-110
2-Methyl-		4	0.060	100	13	BY-104
2,4-Dimethyl-		1	0.100	114	20	BY-107
2,2,4-Trimethyl-		2	0.110	128	19	B-112
2-Hexanone		80	2.700	100	605	C=103
4-Methyl-		3	5.500	114	1081	C=103
5-Methyl-		7	0.190	114	37	C-102
3-Hexanone		16	28.000	100	6272	C-103
2,5-Dimethyl-		1	0.033	128	6	AX-102
2-Heptanone		73	3.100	114	609	C-103
3-Methyl-		3	0.049	128	9	BY-102
4-Methyl-		5	0.100	128	18	BY-107
6-Methyl-		39	12.000	128	2100	C-103
3-Heptanone		68	3.600	114	707	C-103
6-Methyl-		4	0.310	128	54	BY-104
4-Heptanone		18	2.200	114	432	C-103
2-Octanone		63	1.500	128	263	C-103
3-Octanone		4	2.500	128	438	C-103
4-Octanone		7	2.700	128	473	C-103
2-Nonanone		22	10.000	142	1577	C-103
3-Nonanone		1	0.900	142	142	C-103
4-Nonanone		3	0.160	142	25	C-102
5-Nonanone		3	0.015	142	2	BY-104
2-Decanone		8	0.200	156	29	TY-103
4-Decanone		2	0.018	156	3	C-105
5-Decanone		2	0.043	156	6	T-111
2-Undecanone		7	2.800	170	369	C-103
6,10-Dimethyl-		1	0.360	198	41	C-103
3-Undecanone		7	0.800	170	105	BX-103
4-Undecanone		1	0.082	170	11	C-110
5-Undecanone		4	0.130	170	17	BX-103
2-Methyl-		12	1.700	184	207	C-102
2-Dodecanone		3	0.140	184	17	TY-103
3-Dodecanone		15	9.100	184	1108	C-103
4-Dodecanone		1	0.210	184	26	BX-103
5-Dodecanone		3	0.220	184	27	TY-103
2-Tridecanone		6	2.200	198	249	C-101
3-Tridecanone		21	5.400	198	611	C-103
4-Tridecanone		1	0.170	198	19	BX-103
5-Tridecanone		4	0.030	198	3	AX-102
6-Tridecanone		8	0.880	198	100	TY-103
2-Tetradecanone		8	0.110	212	12	TY-103
3-Tetradecanone		3	1.400	212	148	C-103
2-Heptadecanone		2	0.001	254	0.1	BY-105
ALIPHATIC DIKETONES						
2,3-Pentadione		1	0.070	100	16	BY-104
CYCLOALKANONES						
Cyclobutanone		1	0.150	70	48	BY-104
Cyclopentanone						
3-Methyl-		2	0.097	98	22	C-101
2,4-Dimethyl-	(*)	1	0.026	112	5	C-110
2-Methyl-4-(2-methylpropyl)-	(*)	1	0.470	154	68	BY-108
Cyclohexanone		51	0.370	98	85	BY-108
2,2,6-Trimethyl-		2	0.190	140	30	C-101

Table 9a. Ketones (Page 2 of 2)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
3,3,5-Trimethyl-		2	0.210	140	34	C-101
5-Methyl-2-(1-methylethenyl)-Bicyclo[4.1.0]heptan-3-one		2	2.500	152	368	C-204
4,7,7-Trimethyl-		1	0.580	152	85	C-204
ALKENEONES						
3-Buten-2-one		22	3.600	70	1152	C-103
3-Methyl-		2	0.080	84	21	BY-104
3-Penten-2-one						
4-Methyl-	(*)	3	0.086	98	20	AX-102
3-Hexen-2-one	(*)	2	0.490	98	112	AX-102
3-Hepten-2-one						
3-Methyl-	(*)	1	0.140	126	25	AX-102
4-Methyl-	(*)	1	0.040	126	7	TX-118
4-Hepten-3-one						
5-Ethyl-2,4-dimethyl-		1	0.230	168	31	BY-107
1-Octen-3-one		1	0.034	126	6	BY-106
4-Octen-3-one	(*)	3	0.020	126	4	BY-104
2-Nonen-4-one	(*)	1	0.063	140	10	U-106
Z-5,9-Undecadien-2-one						
6,10-Dimethyl-		3	0.007	194	1	C-107
2-Pentanone						
4-Cyclohexylidene-3,3-diethyl-		1	0.170	222	17	BY-108
2-Hexanone						
3-Cyclohexylidene-4-ethyl-		1	0.270	208	29	C-102
AROMATIC KETONES AND QUINONES						
Ethanone						
1-Phenyl-		19	2.400	120	448	C-103
1-Propanone						
1-Phenyl-		1	0.280	134	47	C-101
9H-Fluoen-9-one		2	0.017	180	2	C-110
2,5-Cyclohexdiene-1,4-dione						
2,6-bis(1,1-dimethylethyl)-		8	0.026	220	3	SX-107
Total		**1363**	**222.69**		**57,142**	

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 9b. Ketones Observed in One Tank at Concentration Less Than 0.025 mg/m^3 (Page 1 of 1)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
ALIPHATIC KETONES							
Pentanone	(*)						
4-Hydroxy-4-methyl-		1	0.0180	116	3	TX-118	UKE006-03
2-Hexanone							
6-Methoxy-		1	0.0007	130	0.1	TY-104	29006-00-6
3-Hexanone							
4-Ethyl-		1	0.0034	128	1	AX-102	
5-Methyl-		1	0.0088	114	2	AX-102	623-56-3
2-Heptanone							
4,6-Dimethyl-		1	0.0061	142	1	BY-112	19549-80-5
4-Heptanone							
3-Methyl-		1	0.0200	128	4	B-103	15726-15-5
4-Octanone							
3-Methyl-		1	0.0180	142	3	AX-102	20754-04-5
2-Decanone							
5,9-Dimethyl-		1	0.0240	184	3	C-104	33933-82-3
4-Dodecanone							
11-Methyl-		1	0.0250	198	3	TY-104	29366-35-6
2-Pentadecanone							
6,10,14-Trimethyl-		1	0.0057	268	0.5	BT-105	502-69-2
4-Tetradecanone		1	0.0130	212	1	TY-104	26496-20-8
CYCLOALKANONES							
Cyclobutanone							
2-Ethyl-		1	0.0220	98	5	C-110	10374-14-8
3,3-Dimethyl-		1	0.0047	98	1	TX-118	1192-33-2
2,3,3-Trimethyl-	(*)	1	0.0110	112	2	BY-106	28290-01-9
Cyclopentanone							
trans-3,4-Dimethyl-		1	0.0006	112	0.1	TY-104	19550-73-3
2,2,5-Trimethyl-		1	0.0150	126	3	B-103	4573-09-5
Cyclohexanone							
3-Methyl-		1	0.0210	112	4	T-111	591-24-2
2,6-Dimethyl-	(*)	1	0.0040	126	1	BY-106	16519-68-9
4-Hydroxy-4-methyl-		1	0.0020	128	0.4	C-107	17429-02-6
ALIPHATIC DIONES							
2,5-Hexandione		1	0.0077	114	2	AX-102	110-13-4
ACYCLIC AND CYCLIC ALKENEONES AND RELATED COMPOUNDS							
3-Hexen-2-one							
5-Methyl-	(*)	1	0.0170	112	3	AX-102	5166-53-0
5-Hepten-2-one							
6-Methyl-	(*)	1	0.0070	126	1	C-107	
7-Octen-2-one		1	0.0070	126	1	BY-106	35194-30-?
1-Nonen-3-one							
2-Methyl-		1	0.0060	154	1	C-107	51756-19-5
10-Undecen-4-one							
2,2,6,6-Tetramethyl-	(*)	1	0.0140	224	1	A-102	42565-49-1
3-Cyclopenten-1-one							
2,3,4-Trimethyl-		1	0.0045	124	1	TX-118	83321-16-8
Cyclohexanone							
2,5-Dimethyl-2-(1-methylethenyl)-		1	0.0030	166	0.4	C-107	6711-26-8
2-Cyclohexen-1-one							
4,5-Dimethyl-	(*)	1	0.0250	124	5	BY-102	5715-25-3
4-Ethyl-3,4-dimethyl-	(*)	1	0.0033	152	0	BY-106	17622-46-7
3,4-Undecadien-2,10-dione							
6,6-Dimethyl-		1	0.0020	208	0.2	BY-106	52588-78-0M
E-5,9-Undecadien-2-one							
6,10-Dimethyl-		1	0.0007	194	0.1	AX-103	3796-70-1
AROMATIC KETONES AND QUINONES							
1H-Inden-1-one							
2,3-Dihydro-3,3-dimethyl-		1	0.0030	160	0.4	C-107	26465-81-6
Ethanone							
1-(2,4,5-Trimethylphenyl)-		1	0.0170	162	2	T-111	
1-(3-Methylphenyl)-		1	0.0020	134	0.3	T-107	585-74-0
1-(5,6,7,8-Tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthenyl)-		1	0.0010	258	0.1	C-109	1506-02-1
bis-1,1'-(1,4-phenylene)		1	0.0030	162	0.4	TY-104	1009-61-6
1,4-Cyclohexadienone		1	0.0170	108	4	U-106	637-88-7
Total		**37**	**0.3632**		**60**		

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 10a. Acids

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALKANOIC ACIDS						
Ethanoic		19	0.700	60	261	C-104
Propanoic		4	0.017	74	5	C-108
Butanoic		2	3.300	88	840	C-103
Decanoic		2	0.003	172	0.4	C-111
Dodecanoic		6	0.310	200	35	BY-108
Tetradecanoic		22	4.000	228	393	C-103
12-Methyl-		2	0.010	242	1	C-107
Pentadecanoic		13	2.400	242	222	C-103
Hexadecanoic		30	4.200	256	368	C-103
ALKENOIC ACIDS						
Propenoic		1	4.400	72	1369	C-103
Pentadec-14-enoic	(*)	3	0.042	240	4	BY-107
Hexadec-9-enoic	(*)	14	3.700	254	326	C-103
Z-Octadec-9-enoic		5	0.070	282	6	BY-107
Total		**123**	**23.15**		**3830**	

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 10b. Acids Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Hexanoic Acid	1	0.0040	116	1	C-109	142-62-1
2-Ethyl-	1	0.0020	144	0.3	C-109	149-57-5
Octadecanoic Acid	1	0.0040	284	0.3	C-108	57-11-4
Cyclohexanecarboxylic Acid trans-2-(1,1-Dimethylethyl)-	1	0.0020	170	0.3	C-112	27392-16-1
Total	**4**	**0.0120**		**2**		

Table 11a. Esters

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALKANE ESTERS					
Methanoic Acid Ester					
2-Methylpropyl	1	0.300	102	66	B-103
2-Propenyl	1	4.100	86	1068	C-103
Butyl	5	3.300	102	725	C-103
2,6-Dimethylhept-5-en-2-ol (*)	3	0.370	170	49	BY-108
Ethanoic Acid Ester					
Methyl	2	0.140	74	42	U-103
Ethyl	3	47.000	88	11964	C-103
2-Propenyl	1	4.600	100	1030	C-103
Butyl	9	17.000	116	3283	C-103
Hexadecanyl	3	0.054	284	4	BY-107
Propanoic Acid Ester					
Butyl	1	1.100	130	190	C-103
Octyl	1	0.030	186	4	U-106
2-Methylpropanoic Acid Ester					
Butyl	1	0.026	144	4	AX-102
Butanoic Acid Ester					
Butyl	6	2.600	144	404	C-103
E-2-Hexenyl	1	0.040	170	5	BY-105
Butanedioic Acid Ester					
Diethyl	1	5.200	174	669	C-103
Hexandioic Acid Ester					
Dioctyl	4	1.600	398	90	C-103
2-Ethylhexyl-	1	0.030	286	2	B-103
bis(2-Ethylhexyl)	1	0.064	398	4	S-105
E-Hexa-2-enoic Acid Ester					
E-2-Hexenyl	1	0.031	196	4	C-102
Heptanoic Acid Ester					
Butyl	2	0.009	186	1	C-105
Tetradecanoic Acid Ester					
1-Methylethyl	8	2.000	270	166	C-103
Butyl	4	2.500	284	197	C-103
Hexadecanoic Acid Ester					
1-Methylethyl	33	0.440	298	33	BY-108
Octadecanoic Acid Ester					
Butyl	1	0.029	340	2	C-105
BENZENE ESTERS					
1,2-Benzenedicarboxylic Acid Ester					
Diethyl	11	1.300	222	131	U-106
Dibutyl	2	0.006	278	0.5	C-104
Butyl Cyclohexyl	1	0.080	304	6	S-110
PHOSPHATE ESTERS					
Butylphosphoric Acid Ester					
Dibutyl	13	0.780	250	70	C-103
Phosphoric Acid Ester					
Tributyl	29	6.400	266	539	C-103
Total	**150**	**101.13**		**20,752**	

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 11b. Esters Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
ALKANE ESTERS							
Methanoic Acid Ester							
Methyl		1	0.0020	60	1	T-107	107-31-3
Ethanoic Acid Ester							
1-Hepten-1-ol		1	0.0230	156	3	A-103	35468-97-4
Oxoethanoic Acid Ester							
Butyl		1	0.0014	130	0.2	AX-103	
Propanoic Acid Ester							
2-Propyn-1-ol		1	0.0060	112	1	U-112	1932-92-9
Butanoic Acid Ester							
1-Methylpropyl		1	0.0010	144	0.2	T-107	819-97-6
Hexyl		1	0.0010	172	0.1	C-109	2639-63-6
2-Oxo-3-methylpentanoic Acid Ester							
Methyl		1	0.0230	144	4	U-106	3682-42-6
Pentanoic Acid Ester							
Hexyl		1	0.0170	186	2	B-103	1117-59-5
2-Hexenoic Acid Ester							
4-Methylpentyl	(*)	1	0.0130	198	1	U-103	69687-91-8
2-Ethylhexanoic Acid Ester							
Butyl		1	0.0110	200	1	AX-102	68443-63-0
Hexandioic Acid Ester							
Butyl		1	0.0026	202	0.3	C-106	111-06-8
bis(1-Methylpropyl)		1	0.0020	258	0.2	C-107	38447-22-2
Pentadecanoic Acid Ester							
Butyl		1	0.0082	298	1	C-106	35996-97-5
Hexadecanoic Acid Ester							
2,3-Dihydroxypropyl		1	0.0040	330	0.3	C-107	542-44-9
Butyl		1	0.0026	312	0.2	C-106	111-06-8
E-9-Octadecenoic Acid Ester							
Methyl		1	0.0085	296	1	C-107	1937-62-8
a-Hydroxybenzeneacetic Acid Ester							
Methyl		1	0.0079	166	1	SX-103	20698-91-3
Ethyl		1	0.0140	180	2	SX-106	774-40-3
BENZENE ESTERS							
1,2-Benzenedicarboxylic Acid Ester							
Butyl 2-Methylpropyl		1	0.0110	278	1	C-108	17851-53-5
Butyl 2-ethylhexyl		1	0.0090	334	1	C-104	85-69-8
bis(2-Ethylhexyl)		1	0.0050	390	0.3	C-108	117-81-7
4-(1,1-Dimethylethyl)benzoic Acid Ester							
Methyl		1	0.0045	192	1	C-108	26537-19-9
Total		**22**	**0.1777**		**21**		

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 12a. Nitriles

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALKANE NITRILES						
Acetonitrile		205	23.400	41	12784	C-103
Propanenitrile		163	13.000	55	5295	C-103
2-Methyl-		2	0.060	69	19	BY-104
2,2-Dimethyl-		3	0.077	83	21	TX-111
Butanenitrile		127	7.900	69	2565	C-103
Pentanenitrile		114	4.000	83	1080	C-103
Hexanenitrile		117	3.700	97	854	C-103
Heptanenitrile		51	3.200	111	646	C-103
Octanenitrile		23	1.900	125	340	C-103
Nonanenitrile		19	0.920	139	148	C-103
Decanenitrile		2	0.011	153	2	U-106
Undecanenitrile		2	0.002	167	0.3	TY-104
Tridecanenitrile		1	0.089	181	11	BY-107
ALKENE NITRILES						
2-Propenenitrile		3	0.027	53	11	TX-118
2-Methyl-		1	0.110	67	37	C-101
2-Butenenitrile	(*)	3	0.017	55	7	C-110
3-Butenenitrile	(*)	2	0.062	55	25	BY-106
CYCLOALKANE NITRILES						
Cyclopropanenitrile		2	0.022	53	9	C-107
AROMATIC NITRILES						
Benzonitrile		5	0.075	103	16	C-110
Total		**845**	**58.57**		**23,871**	

Notes
(*) The positional, geometrical or stereo isomer has not been defined.

Table 12b. Nitriles Observed in One Tank at Concentration Less Than 0.025 mg/m^3

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Acetonitrile Hydroxy-		1	0.0029	57	1	TY-104	107-16-4
Undecanenitrile		2	0.0022	167	0.3	TY-104	2244-07-7
2,4-Pentadienenitrile	(*)	1	0.0030	79	1	U-112	1615-70-9
Total		**4**	**0.0081**		**2**		

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 13a. Amines and Amides

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ALIPHATIC AMINES						
Methanamine						
N, N-Dimethyl-		1	1.700	59	645	C-103
N-(1-Methylbutylidene)-	(*)	5	0.580	99	131	BY-107
Butanamine						
N-Ethylidene-	(*)	2	0.035	59	13	U-106
1-Pentanamine						
5-Hydroxy-		2	0.003	103	1	TY-101
CYCLIC ALIPHATIC AMINES						
Aziridine						
2-Methyl-		3	0.140	57	55	S-102
2-Ethyl-		5	0.180	71	57	A-101
Pyrrolidine		2	2.100	71	663	C-103
4-Piperidinemethanol						
1-Methyl-		1	0.043	129	7	U-106
1,3,5,7-Tetraazatri(3.3.1.1(3,7))decane		9	0.032	140	5	TY-101
AROMATIC AMINES						
Benzeneamine						
N-Phenyl		10	0.230	169	30	BY-108
ALIPHATIC AMIDES						
Cyanamide						
Dimethyl-		1	0.130	70	42	U-106
Formamide		3	0.008	45	4	BY-112
N-(2-Methylpropyl)-		1	0.026	101	6	BY-106
N-Butyl-		2	0.060	101	13	A-101
Acetamide		2	0.084	59	32	AX-102
N,N-Dimethyl-		2	0.050	87	13	C-105
Butanamide		3	0.077	87	20	AX-102
Octanamide						
N-(2-Hydroxyethyl)-		2	0.022	187	3	A-103
CYCLIC ALIPHATIC AMIDES						
2-Pyrrolidinone		5	0.960	85	253	C-103
1-Methyl-		1	0.110	99	25	BY-109
2,5-Pyrrolidenedione						
1-Methyl-		2	0.028	113	6	C-108
Total		**64**	**6.60**		**2024**	

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 13b. Amines and Amides Observed in One Tank at a Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
ACYCLIC ALIPHATIC AMINES						
Methanamine						
N-(1-Methylhexylididene)-	1	0.0130	127	2	C-104	22058-71-5
N-(4-Hydroxy-2-methoxyphenyl)-	1	0.0210	167	3	T-107	1196-92-5
Propanamine						
3-Cyano-	1	0.0023	84	1	T-107	151-18-8
1-Butanone						
4-(Dimethylamino)-1-phenyl-	1	0.0160	215	2	C-110	3760-63-2
1-Octadecanamine						
N,N-Dimethyl-	1	0.0040	297	0.3	TY-104	124-28-7
1,4-Butanediamine	1	0.0012	88	0.3	TY-104	110-60-1
ACYCLIC ALIPHATIC AMIDES						
Acetamide						
N-Methyl-	1	0.0012	73	0.4	TY-104	79-16-3
Butanamide						
N-Hexyl-	1	0.0004	171	0.1	AX-103	10264-17-2
Nonanamide	1	0.0080	157	1	TY-104	1120-07-6
Decanamide						
N-(2-Hydroxyethyl)-	1	0.0055	215	1	TY-104	
Dodecanamide						
N-(2-Hydroxyethyl)-	1	0.0078	243	1	TY-104	142-78-9
Hexadecanamide	1	0.0030	255	0.3	C-108	629-54-9
BENZENE DERIVATIVES						
Benzeneamine						
2-Ethyl-	1	0.0083	121	2	A-102	578-54-1
Benzamide						
N-Methyl-	1	0.0020	135	0	C-107	613-93-4
CYCLIC AMIDES						
3-Piperidinecarboxamide						
N-Methyl-	1	0.0094	142	1	SX-106	5115-98-0
Total	**15**	**0.1031**		**14**		

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

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
NITROUS ACID ESTERS					
Alcohol Component					
Methyl	11	0.870	61	319	B-103
Butyl	6	0.760	103	165	A-101
NITRIC ACID ESTERS					
Alcohol Component					
Methyl	14	0.200	77	58	C-112
Ethyl	23	0.450	91	111	BX-103
1-Methylethyl	4	0.150	105	32	C-102
Propyl	28	1.100	105	235	TY-105
2,2-Dimethyl-	6	0.170	133	29	AX-102
Butyl	27	0.810	119	152	TY-105
3-Methyl-	5	0.250	133	42	BX-103
Pentyl	12	0.310	133	52	B-103
Hexyl	12	0.620	147	94	BX-103
Heptyl	3	0.039	161	5	TX-111
Diol and Triol Component					
1,3-Propanediol	1	13.000	178	1636	C-204
1,4-Butanediol	4	2.100	192	245	C-103
1,5-Pentanediol	4	0.028	206	3	B-103
Propane-1,2,3-triol					
1-Nitrate	1	0.160	149	24	C-204
1,3-Dinitrate	2	0.077	192	9	TX-106
NITRO COMPOUNDS					
Methane					
Nitro-	4	0.140	61	51	U-112
Trinitrofluoro-	2	0.110	169	15	BX-103
Propane					
1-Nitro-	2	0.130	89	33	TY-105
2-Nitro-2-methyl-	26	0.160	103	35	TX-110
Butane					
1-Nitro-	6	1.800	103	391	C-204
Benzene					
1-Nitro	2	0.015	123	3	TX-118
1-Nitro-4-methyl-	2	0.002	137	0.3	T-107
NITROSO COMPOUNDS					
Nitrosomethane	1	0.190	45	95	TX-118
4-Nitrosomorpholine	1	0.050	100	11	U-108
Methanamine					
N-Methyl-N-nitroso-	26	0.270	74	82	U-108
Total	**235**	**23.961**		**3928**	

Table 14b. Nitrous and Nitric Acid Esters, Nitrous and Nitro Compounds Observed in One Tank at a Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
NITRIC ACID ESTERS						
Nitrate						
2-Methylpropyl	1	0.0022	119	0.4	TX-105	543-29-3
Nonyl	1	0.0014	189	0.2	TY-104	20633-13-0
Decyl	1	0.0086	203	1	TX-118	2050-78-4
NITRO COMPOUNDS						
Propane						
2-Methyl-1-nitro	1	0.0090	103	2	U-112	625-74-1
Butane						
2-Nitro-	1	0.0055	103	1	U-112	600-24-8
Z-1-Nitropropene	1	0.0080	87	2	TY-104	27675-36-1
BENZENE DERIVATIVES						
Benzene						
1-Nitro-4-chloro-	1	0.0053	134	1	C-107	100-00-5
Total	**7**	**0.0400**		**8**		

Table 15a. Heterocycles (Page 1 of 1)

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
Oxirane		1	0.052	44	26	TY-104
Ethyl		1	0.270	72	84	B-103
Ethenyl-		4	2.500	70	800	BY-108
cis-2-Ethyl-3-propyl		1	0.160	114	31	BX-104
Furan		9	9.700	68	3195	C-103
2-Methyl-		2	3.700	82	1011	C-103
2-Propyl-		2	0.046	110	9	BY-109
2-Pentyl-		2	0.016	138	3	AX-103
2-Heptyl-		1	0.330	166	45	BY-108
2,5-Dimethyl-		1	0.040	96	9	BY-104
2-Ethyl-5-methyl-		2	0.050	110	10	AX-102
2,3-Dihydrofuran		5	0.050	70	16	C-110
2,5-Dihydrofuran		5	2.700	70	864	C-103
Tetrahydrofuran		166	16.000	72	4978	C-103
2,5-Diethyl-	(*)	1	0.110	128	19	A-101
2,5-Dipropyl-	(*)	2	0.007	156	1	TY-104
Dihydro-2(3H)-Furanone		6	3.500	84	933	C-103
5-Methyl-		4	0.044	98	10	AX-102
5-Ethyl-		9	0.089	112	18	U-106
5-Propyl-		7	0.011	126	2	C-104
5-Butyl-		4	0.006	140	1	TY-104
5-Hexyl-		2	0.006	168	1	C-104
3,5-Dimethyl-		2	0.710	112	142	C-102
Benzofuranone						
3a,4,5,6-tetrahydro-3a,6,6-trimethyl-		6	0.730	188	87	BY-108
Tetrahydrofuranmethanol		1	0.075	102	16	C-102
Furanacetaldehyde						
alpha-propyl		1	0.200	152	29	BY-107
1,4-Dioxane		8	0.060	88	15	S-102
2,3-Dioxabicyclo[2.2.2]oct-5-ene						
1-Methyl-4-(1-methylethyl)-		1	0.400	188	48	C-103
2,2-Bioxepane		6	0.054	72	17	AX-102
2H-Pyran-2-one						
Tetrahydro-5,6-dimethyl-		5	1.200	128	210	BY-108
1H-Pyrrole		2	0.012	67	4	BY-106
Pyridine		96	0.430	79	122	BY-108
2-Methyl-		1	0.061	93	15	C-104
3-methyl-		5	0.150	93	36	C-101
4-Methyl-		5	0.037	93	9	C-105
2-Ethyl-		2	0.011	107	2	AX-102
2,4-Dimethyl-		3	0.500	107	105	C-103
2,5-Dimethyl-		1	0.089	107	19	C-104
5-Ethyl-2-methyl-		2	0.014	121	3	C-104
1,2,3,6-Tetrahydropyridine		2	0.110	83	30	U-106
Pyrimidine		4	0.390	80	109	U-102
4-Methyl-		1	0.038	94	9	TX-111
Pyrazine		40	0.390	80	109	U-102
Methyl-		9	0.023	94	5	TX-111
Ethyl-		4	0.032	108	7	TX-111
2,3-Dimethyl-		3	0.015	108	3	A-103
1H-1,2,4-Triazole		2	0.027	69	9	U-103
1-Ethyl-		1	0.130	97	30	BY-105
1H-Pyrazole						
3-Methyl-		3	0.230	82	63	BX-104
4,5-Dihydro-1H-pyrazole						
5-Methyl-		1	0.067	96	16	U-106
4,5-Dihydrooxazole						
2-Methyl-		8	0.062	99	14	U-106
2-Propyl-		3	0.047	127	8	S-102
2-Oxazolidinone						
5-Methyl-3-(2-propenyl)-	(*)	4	0.067	141	11	U-106
Isothiazole		2	0.003	97	1	C-112
Benzothiazole		4	0.060	135	10	BY-106
2-Phenyl-		4	0.062	211	7	SX-106
Total		**479**	**45.872**		**13,385**	

Note
(*) The positional, geometrical or stereo isomer has not been defined.

Table 15b. Heterocycles Observed in One Tank at a Concentration Less Than 0.025 mg/m^3

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Oxirane							
(1-Methylbutyl)-		1	0.0024	114	0.5	S-111	53229-39-3
2-Methyl-2-pentyl-		1	0.0160	128	3	C-104	53907-75-8
1,3,6-Trioxocane		1	0.0083	90	2	U-112	1779-19-7
Furan							
2-Octyl-		1	0.0065	180	1	BY-106	4179-38-8
2-(2-Methyl-6-oxoheptyl)-	(*)	1	0.0045	194	1	C-105	51595-87-0
2-(3-Oxo-3-phenylprop-1-enyl)-	(*)	1	0.0051	198	1	SX-106	717-21-5
2,3-Dihydrofuran							
3-(1,1-Dimethylethyl)-		1	0.0030	126	1	BY-105	34314-82-4
4-(1-Methylpropyl)-		1	0.0055	126	1	AX-102	34379-54-9
Tetrahydrofuran							
trans-2,4-Dimethyl-		1	0.0140	100	3	B-103	39168-02-0
Dihydro-2(3H)-Furanone							
4,4-Dimethyl-		1	0.0060	114	1	BY-112	13861-97-7
5-Ethenyl-5-methyl-		1	0.0025	126	0.4	SX-106	1073-11-6
5-Ethyl-5-methyl-		1	0.0079	128	1	TX-105	2865-82-9
5-Pentyl-		1	0.0170	156	2	AX-102	104-61-0
Dihydro-2,5-Furandione		1	0.0089	100	2	SX-103	108-30-5
2,4(3H,5H)-Furandione							
3-Methyl-		1	0.0180	114	4	AX-102	1192-51-4
Tetrahydrofuranmethanol							
trans-5-Methyl-		1	0.0034	116	1	TX-118	54774-28-6
Acetic acid ester		1	0.0030	144	0.5	T-107	637-64-9
1,3-Dioxane							
4,4-Dimethyl-		1	0.0090	116	2	C-105	766-15-4
1,3-Benzodiox-2-one		1	0.0023	150	0.3	C-107	20192-66-9
2H-Pyran							
3,4-Dihydro-2-carboxaldehyde		1	0.0079	112	2	A-102	100-73-2
Tetrahydro-2-(1,1-Dimethylethoxy)-		1	0.0050	158	1	TY-104	1927-69-1
2H-Pyran-2-one							
Tetrahydro-6-hexyl-		1	0.0027	184	0.3	S-111	710-04-3
Tetrahydro-6,6-dimethyl-		1	0.0030	128	1	C-112	2610-95-9
Dihydro-2H-Pyran-3(4H)-one		1	0.0045	98	1	C-107	23462-75-1
1H-Pyrrole							
2,5-Dimethyl-		1	0.0110	95	3	SX-106	625-84-3
Pyridine							
3,4-Dimethyl-		1	0.0071	107	1	S-111	583-58-4
2,6-Dimethyl-		1	0.0120	107	3	C-104	108-48-5
2,3,6-Trimethyl-		1	0.0007	121	0.1	TY-104	1462-84-6
Pyrazine							
2,5-Dimethyl-		1	0.0019	110	0.4	S-111	123-32-0
2,5-Dimethyl-3-(3-methylbutyl)-		1	0.0100	178	1	C-104	18433-98-2
4H-1,2,4-Triazole							
3-Amino-4-ethyl-		1	0.0095	112	2	C-108	42786-06-1
1H-Pyrazole							
1-Methyl-		1	0.0066	82	2	TX-118	930-36-9
4,5-Dihydro-1H-pyrazole							
4,5-Dimethyl-		1	0.0240	98	5	U-106	28019-94-5
5-Propyl-		1	0.0230	112	5	U-103	75011-90-4
1H-Pyrrolo(2,3-b)pyridine							
6-Amino-2,3-diphenyl-		1	0.0160	285	1	SX-106	UHC000-11
Hexahydro-1H-Azepin-1-amino							
N-Ethylidenehexa-		1	0.0083	140	1	C-112	75268-01-8
1H-Imidazole							
2-Methyl-		1	0.0016	82	0.4	TY-104	693-98-1
1H-Indole							
2-Phenyl-		1	0.0056	198	1	SX-106	948-65-2
1-Pyrrolidinamine							
2-(Methoxymethyl)-		1	0.0018	130	0.3	TY-104	59983-39-0
1-Pyrrolidinecarboxylaldehyde		1	0.0006	99	0.1	TY-104	3760-54-1
4(3H)-Pyrimidinone		1	0.0220	96	5	BY-102	51953-17-4
Total		**41**	**0.3281**		**62**		

(*) The positional, geometrical or stereo isomer has not been defined.

Table 16a. Sulfur Compounds

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
THIOLS					
1-Propanethiol					
2,2-Dimethyl-	1	0.031	104	7	C-105
SULFONES					
Propane					
2-[(1,1-Dimethylethyl)sulfonyl]-2-methyl-	3	0.005	178	1	S-111
Benzene					
Ethylsulfonyl-	1	0.088	170	12	C-109
THIOCARBOXYLIC ACIDS, ESTERS AND AMIDES					
Butanethioic Acid Ester					
S-Decyl Ester	3	0.240	260	21	U-106
Benzenesulfonamide					
N-Butyl-	40	1.500	213	158	BY-108
Total	**48**	**1.864**		**197**	

Table 16b. Sulfur Compounds Observed in One Tank at a Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Thiophene						
2-Methoxy-5-methyl-	1	0.023	128	4	C-104	31053-55-1
Benzenesulfonamide						
N-Ethyl-N-methyl-	1	0.001	199	0.1	BY-112	80-39-7
N-Hexyl-	1	0.005	241	0.4	C-108	7250-80-8
Total	**3**	**0.029**		**5**		

Table 17a. Silicon Compounds

Compound		Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
SILANES AND SILOXANES						
Silane						
Trimethyl-		1	0.044	74	13	TX-111
Chlorotrimethyl-		7	0.048	109	10	AX-102
Dimethoxydimethyl-		3	0.056	120	10	S-102
Silanol						
Trimethyl-		6	0.035	90	9	A-103
Siloxane		13	1.300			A-103
Cyclotrisiloxane						
Tetramethyl-		1	4.000	194	462	A-103
Hexamethyl-		56	6.300	222	636	C-103
Cyclotetrasiloxane						
Octamethyl-		46	5.400	296	409	C-103
Decamethyl-		1	0.037	324	3	A-103
SILANE ESTERS						
Ethanedioic Acid Ester						
bis(TMS) Ester	(*)	4	0.140	234	13	A-102
2-[(TMS)oxy]benzoic Acid	(*)					
TMS Ester	(*)	18	0.220	270	18	A-103
alpha,4-bis(TMSoxy)benzeneacetic Acid	(*)					
Methyl Ester		2	0.034	326	2	BY-103
TMS Ester	(*)	2	0.007	384	0.4	C-107
alpha-[(TMS)oxy]benzenepropanoic Acid Ester	(*)					
TMS Ester	(*)	1	0.028	310	2	A-102
OTHER SILICON COMPOUNDS						
1-Propanone						
1-[4-((TMS)oxy)phenyl]-	(*)	1	0.039	222	4	S-102
Benzeneethanamine						
N-[Perfluorophenyl]-beta,4-bis[TMSoxy]	(*)	1	0.082	449	4	U-112
Butanamide						
Perfluoro-N-[2-TMSoxy-2-[4-TMSoxy]phenyl]ethyl-	(*)	1	0.180	493	8	U-106
Total		**164**	**17.950**		**1604**	

Note
(*) The trimethylsilyl fragment is designated as TMS in this table.

Table 17b. Silicon Compounds Observed in One Tank at a Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Silane 4,5-Dimethyl-1,4-Cyclohexadiene-1,2-diyl) bis(trimethyl-	1	0.006	252	1	S-111	101300-62-3
bis(TMS)ethane (4-TMSoxyphenyl)- (1)	1	0.004	370	0.2	SX-103	US1000-04
Propanedioic Acid 2-(TMSoxy)-bis(TMS) ester	1	0.004	336	0.2	AX-102	38165-93-4
E-2-Hexenedioic Acid bis(TMS) ester	1	0.009	260	1	SX-106	55494-10-5
Heptasiloxane Hexdecamethyl-	1	0.022	548	1	AX-102	541-01-5
Cyclotrisiloxane Octamethyl-	1	0.014	252	1	SX-107	US1000-09
3,6-Dioxa-2,4,5,7-Tetrasilaoctane 2,2,4,4,5,5,7,7-Octamethyl-	1	0.021	294	2	AX-102	4342-25-0
Total	**7**	**0.079**		**6**		

Table 18a. Other Organic Compounds

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration
ISOCYANATES					
Methane					
Isocyanato-	2	0.046	57	18	U-106
Propane					
2-Isocyanato-	1	0.044	85	12	C-110
HYDRAZINES					
Hydrazine					
1,1-Dimethyl-	4	0.008	60	3	TX-105
Total	**7**	**0.098**		**33**	

Table 18b. Other Organic Compound Observed in One Tank at a Concentration Less Than 0.025 mg/m^3

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppbv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Hydrazine Methyl-	1	0.0028	46	1	TY-101	60-34-4

Table 19. Inorganic Compounds

Compound	Total Number of Observations	Maximum Concentration, mg/m^3	MW	Maximum Concentration, ppmv	Tank with Maximum Concentration	TWINS2 (CAS) Number
Hydrogen	98	115.45	2	1293.0	C-107	1333-74-0
Carbon Monoxide	25	125.00	28	100.0	A-106	630-08-0
Carbon Dioxide	101	3411.96	44	1737.0	B-102	124-38-9
Nitrous Oxide	123	2160.71	44	1100.0	U-102	10024-97-2
Nitric Oxide	51	2.14	30	1.6	C-103	10102-43-9
Nitrogen Dioxide	16	0.43	16	0.6	BY-102	10102-44-0
Ammonia	141	791.56	17	1043.0	BY-108	7664-41-7
Sulfur Oxides	1		60, 84	0.4	C-104	UIN000-01
Carbonyl Sulfide	2	0.07	60	0.03	TY-101	463-58-1
Carbon Disulfide	5	2.70	76	0.8	C-103	75-15-0
Total	**563**	**6610**		**5276**		

Table 20. Tanks with Highest Organic Carbon Content in Dome Space Determined by Total Non Methane Hydrocarbon Content Measurements, GC-MS Analysis of Summa Canisters or TST Samples (PNNL 1999)

Based on TNMHC		Based on SUMMA		Based on TST	
Tank	Concentration, mg/m3	Tank	Concentration, mg/m3	Tank	Concentration, mg/m3
C-103	520	BY-104	210	C-103	2100
BY-108	310	BY-108	170	BY-108	590
C-204	170	C-102	130	C-102	290
BX-104	130	C-101	87	BY-107	170
BY-101	57	BY-107	84	BY-108	100
BX-103	52	BX-103	55	C-101	98
TY-103	51	BY-110	50	BX-104	85
S-102	28	BX-104	49	TY-103	65
BY-102	20	BY-101	47	BY-101	48
TX-111	16	TY-103	43	BY-104	45

Table 21. Summary of Observations

Category	Total Number of Different Compounds	Total Number of Compounds at less than 0.025 mg/m^3	Total Number of Compounds Observed Only Once	Sum of Maximum Concentration of Compounds, ppmv	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	200	46	54	250	30	42	87
Cycloalkanes	151	41	72	8	3	6	30
Alkenes and Alkadienes	146	40	76	38	5	9	32
Alkynes	6	2	4	1	0	0	2
Arenes	45	22	19	8	3	3	13
Halogen Compounds	63	20	18	43	6	9	14
Alcohols, Phenols and Ethers	114	56	58	124	12	13	22
Aldehydes	42	18	15	27	3	3	9
Ketones	116	45	57	57	10	15	29
Acids	17	7	5	4	1	2	7
Esters	51	31	35	21	4	7	12
Nitriles	22	5	5	24	4	6	8
Amines and Amides	36	18	20	2	0	2	4
Nitro and Nitroso Compounds	34	10	11	4	1	1	8
Heterocycles	97	51	55	13	3	6	12
Sulfur Compounds	8	4	5	0.2	0	0	1
Silicon Compounds	23	13	14	2	0	1	3
Miscellaneous Organic Compounds	5	2	3	1	1	1	1
Inorganic Compounds	10	0	1	4000	6	8	9
Total	**1186**	**431**	**527**	**4627**	**92**	**134**	**303**

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