

**Exhaust Emission Profiles for EPA
SPECIATE Database:
Energy Policy Act (EPAAct) Low-Level
Ethanol Fuel Blends and Tier 2 Light-
Duty Vehicles**



EPA

United States
Environmental Protection
Agency



Exhaust Emission Profiles for EPA SPECIATE Database: Energy Policy Act (EPAcT) Low-Level Ethanol Fuel Blends and Tier 2 Light- Duty Vehicles

Assessment and Standards Division
Office of Transportation and Air Quality
U.S. Environmental Protection Agency



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1.0 Introduction

1.1 Background

To model the impact of air pollutant emissions, speciation profiles are used to distribute individual chemical compounds in total volatile organic compound (VOC) emissions into emission estimates for individual species. The EPA maintains a database of VOC and particulate matter (PM) speciation profiles for various emission sources including mobile sources. This database, called SPECIATE,¹ maintains the record of each profile including its referenced source, testing methods, a subjective rating of the quality of the data, and other detailed data that allow researchers to decide which profile is most suitable for model input. These profiles are used in air quality modeling runs such as those done with the CMAQ (Community Multi-scale Air Quality) model.

Existing SPECIATE profiles become outdated as mobile source emission standards change and as newer and stricter standards result in more stringent control technologies. Transportation fleets are expected to begin using renewable fuels at an increasing rate, and the use of ethanol in gasoline fuel blends will affect the speciation of hydrocarbons in both exhaust and evaporative emissions. In addition, passenger cars and trucks started meeting Tier 2 emission standards with model year 2004. Older speciation profiles do not fully represent this change in technology. The fuel type and fleet turnover changes provide the basis for the development of new passenger car and truck SPECIATE profiles.

Exhaust emission profiles were recently updated for pre-Tier 2 vehicles running on E0 (gasoline without ethanol) based on data from a large cooperative test program in Kansas City, Missouri in which EPA participated.² An E10 (gasoline with 10% ethanol) profile was developed by adjusting the E0 profile, based on expected changes in a subset of chemical species due to addition of ethanol to gasoline. A pre-Tier 2 vehicle profile was also updated for vehicles running on E85 (gasoline with 85% ethanol) using data from an EPA Office of Research and Development program testing light-duty vehicles on ethanol gasoline blends.²

This project examined only exhaust emission profiles. Evaporative emission profiles are being updated in a separate EPA program using information from the Coordinating Research Council. However, these updated evaporative emission profiles may not be available for another year or two. In addition, another EPA program is currently characterizing and quantifying the hydrocarbon components associated with PM emissions. Data from higher level ethanol blends (such as E85) are being obtained separately.

1.2 Purpose of the Project

Exhaust emission profiles from Tier 2 light-duty vehicles with 0%, 10% and 15% ethanol-blended gasoline were developed by ENVIRON International Corporation under EPA Contract

¹ SPECIATE 4.0 Database. <http://www.epa.gov/ttn/chief/software/speciate/index.html>

² ENVIRON International Corporation. 2008. Emission profiles for EPA SPECIATE database. EPA Contract No: EP-C-06-094.

EP-D-07-102 (Work Assignment Number 1-09).³ These profiles were composites based on individual vehicle test data from a program designed to collect data from Tier 2 light-duty vehicles running on low-level ethanol fuel blends.⁴ The program was developed by EPA's Office of Transportation and Air Quality to meet the requirements of the Energy Policy Act (EPA Act) of 2005. Details for underlying test data are provided in Section 2.1 below. After the contract was completed, EPA re-calculated the exhaust emission profiles using an alternate weighting system which is described below. This weighting system uses as an input the distances driven in the LA92 test cycle, since this is the test cycle used to generate the data. ENVIRON used a weighting system that attempts to make the emissions data relevant for comparison to other programs in which the FTP cycle was used to generate the exhaust data.

After recalculating the profiles with the LA92 weighting procedure, EPA made adjustments to the aromatic composition of the E0 and E10 profiles. Blending procedures used on the E0 and E10 fuels affected the aromatic composition in a manner inconsistent with real-world fuels. The EPA normalized the profile percents of aromatic compounds in the E0 and E10 profiles using profiles developed with an in-use gasoline (Kansas City test program).² This adjustment did not affect the total percentage of aromatics in the exhaust but rather the relative composition of one aromatic compound to another (such as the relative proportion of toluene versus xylenes).

This report describes the LA92 weighting and adjustment procedures and presents the resulting exhaust emissions profiles to be used in the SPECIATE database.

2.0 Methods

2.1 Exhaust Emissions Data

Exhaust emission profiles were developed with EPA's Office of Transportation and Air Quality EPA Act Phase I Testing Data.⁴ Testing and data collection were conducted by the Southwest Research Institute. Data included emission factors (mg/mi) for speciated compounds from three bags collected over the LA92 drive cycle with Bags 1, 2, and 3 representing 1.19 mi, 8.63 mi, and 1.19 mi, respectively. Speciated compounds included volatile organic compounds (VOCs), aldehydes, ketones, and alcohols. Nineteen Tier 2 light-duty vehicles were tested with multiple runs across three fuels: E0, E10, E15 (gasoline with 15% ethanol). Fuel properties are shown in Table 1. Data from all three bags were collected for three vehicles only; these data were used to create composite emission factors and subsequent composite profiles (Section 2.2 below). The three vehicles were all model year 2008 and included one I-4 compact sedan, one V-6 mini-van, and one V-8 full-size truck. At least two test runs were performed for each vehicle, and three

³ ENVIRON International Corporation. 2008. Emission profiles for EPA SPECIATE database, Part 2: EPA Act fuels. EPA Contract No: EP-D-07-102.

⁴ US EPA. 2008. EPA Act Phase I Testing: Comprehensive Gasoline Light-Duty Exhaust Fuel Effects Test Program to Cover Multiple Fuel Properties and Two Ambient Test Temperatures. EPA Contract: EPC-07-028EPA. Southwest Research Institute, San Antonio, TX

test runs were performed in some cases. E0, E10, and E15 fuel types included 9, 6, and 7 test runs, respectively, across all three vehicles.

Table 1: EPA Phase I testing fuel properties.

Test	Units	E0	E10	E15
RVP	psi	9.0	9.0	9.0
T50	°F	215	211	180
T90	°F	323	319	313
Aromatics	vol%	29.5	24.7	25.9
Benzene	vol%	0.46	0.68	0.71
Toluene	vol%	4.59	4.39	6.37

2.2 Calculation of Composite Profiles

Composite emission factors (EFs), representing a composite of cold start (Bag 1), hot start (Bag 3), and hot-stabilized operation (Bag 2) were calculated using straight-weighting, i.e., bags were multiplied by the LA92 distances without applying additional weighting factors. Equation 1 below was used to determine composite values for the three vehicles with EFs from Bags 1, 2, and 3. An EF reported as non-detect (ND) was treated as a zero.

$$EF_{\text{Composite}} = \frac{(EF_{\text{Bag1}} \times 1.19\text{mi}) + (EF_{\text{Bag2}} \times 8.63\text{mi}) + (EF_{\text{Bag3}} \times 1.19\text{mi})}{(1.19\text{mi} + 8.63\text{mi} + 1.19\text{mi})} \quad \text{Eq. 1}$$

Where:

$EF_{\text{Composite}}$ = Composite emission factor in mg/mi

EF_{Bag1} = Bag 1 emission factor in mg/mi

EF_{Bag2} = Bag 2 emission factor in mg/mi

EF_{Bag3} = Bag 3 emission factor in mg/mi

Individual compound EFs were flagged as outliers for a given test run if their values were outside the bounds of 3.5 standard deviations from the mean. No outlier test runs were determined for the composite profiles. The percentage of each compound in a test run was then calculated by dividing its composite EF by the sum of all EFs for that test run. Percentages for a given compound were averaged across all test runs per fuel type.

2.3 Adjustment of E0 and E10 profiles with an In-Use Gasoline

The aromatic composition of the E0 and E10 fuels, used to develop the E0 and E10 emission exhaust profiles, was found upon speciation of the fuel blends to be inconsistent with the specific aromatic compounds found in real-world fuels. EPA adjusted the profile percents of aromatic compounds in the E0 and E10 profiles using the E0 and E10 profiles developed with the Kansas City test program, which uses an in-use gasoline.² The ratio of each aromatic compound to total

aromatic composition of the exhaust emission profile was determined for the Kansas City E0 and E10 profiles and applied to the respective E0 and E10 profiles developed in this program. The resulting adjusted E0 and E10 profiles, as well the unadjusted E15 profile, were then presented for inclusion into SPECIATE following the assignment of SPECIATE ID numbers.

2.4 Assignment of SPECIATE Identification Numbers

SPECIATE4¹ identification numbers were matched to compounds in the exhaust emission profiles using CAS numbers and SPECIATE4 IDs in the Spec4Asn-8-10-06.xls file created by William Carter (Appendix A). Compounds without CAS numbers were matched with ENVIRON's SPECIATE4 IDs.² For compounds that did not have a one-to-one match with a SPECIATE4 compound, ENVIRON used the most similar SPECIATE4 compound. Table 2 lists the SPECIATE substitutions made by ENVIRON.

Table 2: SPECIATE surrogates used by ENVIRON.²

Composite Exhaust Profiles	
Original Chemical Analysis	SPECIATE Substitution
Dimethylbenzaldehyde	2,5-Dimethylbenzaldehyde
Unidentified C9-C12+	C9-C12 isoalkanes
Cold Start (Bag 1) Profiles	
Original Chemical Analysis	SPECIATE Substitution
3,4 Dimethylcumene	1,3-dimethyl-4-isopropylbenzene
2-Methylbutylbenzene (Sec Amylbenzene)	1-Methyl-2-n-butylbenzene
1-Trans-2-Cis-4-Trimethylcyclopentane	1,2,3-trimethylcyclopentane
Tert-1-Butyl-4-Ethylbenzene	1-(1,1-dimethylethyl)-3,5-dimethylbenzene
Methylpropylbenzene (Sec Butylbenzene)	(1-Methylpropyl)benzene

All Carter-matched SPECIATE4 IDs were checked against ENVIRON's SPECIATE4 IDs. Two compounds showed different SPECIATE4 IDs: 1-trans-2-cis-3-trimethylcyclopentane and 2-methylbutylbenzene (sec amylbenzene). The fractions of both compounds in the profile were less than 0.01%. The Carter SPECIATE4 ID (1537) was chosen for 1-trans-2-cis-3-trimethylcyclopentane as both the Carter and ENVIRON ID code appear to map to same mechanism species. ENVIRON's SPECIATE4 ID (83) was chosen for 2-methylbutylbenzene (sec amylbenzene) since the Carter ID code was already used in a cold start profile for n-pentbenzene.

3.0 Results

3.1 Composite Profiles

The final composite profiles for E0, E10, and E15 are presented in Tables 3, 4 and 5. Table 3 shows percentages of compounds grouped by class. Table 4 shows percentages for five compounds of interest. Table 5 shows the complete profiles with all compounds and includes CAS and SPECIATE ID numbers. These profiles will be released in the next update of the SPECIATE database, SPECIATE 4.2 (anticipated profile numbers: 8756-8758).

Table 3: Composite profile percentages by compound class.

Compound	E0	E10	E15
Paraffins	46.98%	44.38%	47.15%
Olefins	22.53%	22.33%	21.64%
Oxygenate	0.00%	0.00%	0.00%
Aromatics	24.93%	25.02%	22.00%
Aldehydes	2.22%	2.94%	3.75%
Ketones	0.43%	0.36%	0.51%
Alcohols	2.91%	4.98%	4.95%
Sum	100.00%	100.00%	100.00%

Table 4: Composite profile percentages of selected compounds.

Compound	E0	E10	E15
1,3-Butadiene	1.16%	0.89%	0.51%
Acetaldehyde	0.45%	1.61%	2.23%
Acrolein	0.09%	0.07%	0.08%
Benzene	3.43%	3.78%	3.82%
Formaldehyde	0.93%	0.87%	1.07%

Table 5: Composite profile percentages with all compounds.

Compound	CAS Number	Specie ID	E0	E10	E15
METHANE	74-82-8	529	16.291%	17.358%	17.010%
ETHANE	74-84-0	438	2.617%	2.704%	2.776%
ETHYLENE	74-85-1	452	10.477%	10.053%	9.920%
PROPANE	74-98-6	671	0.133%	0.151%	0.106%
PROPYLENE	115-07-1	678	4.059%	3.991%	3.809%
ACETYLENE	74-86-2	282	1.445%	1.647%	1.341%
BUTANE	106-97-8	592	3.526%	3.554%	2.247%
TRANS-2-BUTENE	624-64-6	737	0.492%	0.358%	0.342%
1-BUTENE	106-98-9	64	0.731%	0.683%	0.641%
2-METHYLPROPENE (ISOBUTYLENE)	115-11-7	497	1.623%	1.918%	1.827%
2,2-DIMETHYLPROPANE (NEOPENTANE)	463-82-1	127	0.000%	0.000%	0.000%
1,3-BUTADIENE	106-99-0	46	1.157%	0.891%	0.512%
CIS-2-BUTENE	590-18-1	367	0.360%	0.289%	0.277%
2-METHYLBUTANE (ISOPENTANE)	78-78-4	508	2.188%	0.669%	7.214%
PENTANE	109-66-0	605	0.485%	0.124%	0.563%
2-METHYL-1,3-BUTADIENE	78-79-5	511	0.174%	0.102%	0.461%
TRANS-2-PENTENE	646-04-8	742	0.238%	0.046%	0.088%
3,3-DIMETHYL-1-BUTENE	558-37-2	203	0.000%	0.000%	0.006%
CIS-2-PENTENE	627-20-3	371	0.135%	0.218%	0.213%
2-METHYL-2-BUTENE	513-35-9	185	0.510%	0.000%	0.118%
CYCLOPENTADIENE	542-92-7	48	0.237%	0.135%	0.153%
2,2-DIMETHYLBUTANE	75-83-2	122	0.017%	0.018%	0.059%
CYCLOPENTENE	142-29-0	391	0.132%	0.064%	0.034%
4-METHYL-1-PENTENE	691-37-2	258	0.000%	0.050%	0.000%
3-METHYL-1-PENTENE	760-20-3	232	0.000%	0.000%	0.031%
CYCLOPENTANE	287-92-3	390	0.080%	0.000%	0.053%
2,3-DIMETHYLBUTANE	79-29-8	136	0.537%	0.268%	0.309%
2-METHYLPENTANE	107-83-5	199	0.949%	1.010%	0.775%
4-METHYL-TRANS-2-PENTENE	674-76-0	262	0.000%	0.000%	0.000%
3-METHYLPENTANE	96-14-0	248	0.610%	1.135%	0.436%
2-METHYL-1-PENTENE	763-29-1	184	0.000%	0.541%	0.422%
1-HEXENE	592-41-6	78	0.000%	0.541%	0.422%
HEXANE	110-54-3	601	0.279%	2.911%	0.883%
UNIDENTIFIED C6	#N/A	1999	0.115%	0.023%	0.069%
CIS-3-HEXENE	7642-09-3	372	0.000%	0.032%	0.000%
TRANS-2-HEXENE	4050-45-7	740	0.081%	0.033%	0.017%
3-METHYL-TRANS-2-PENTENE	616-12-6	239	0.095%	0.018%	0.000%
2-METHYL-2-PENTENE	625-27-4	187	0.072%	0.018%	0.015%
3-METHYLCYCLOPENTENE	1120-62-3	242	0.000%	0.000%	0.000%
CIS-2-HEXENE	7688-21-3	369	0.000%	0.000%	0.006%
3-METHYL-CIS-2-PENTENE	922-62-3	236	0.123%	0.000%	0.006%
2,2-DIMETHYLPENTANE	590-35-2	126	0.154%	0.400%	0.261%
METHYLCYCLOPENTANE	96-37-7	551	0.151%	0.386%	0.259%
2,4-DIMETHYLPENTANE	108-08-7	152	0.402%	0.273%	0.217%
2,2,3-TRIMETHYLBUTANE	464-06-2	112	0.020%	0.018%	0.000%

Table 5 (cont.): Composite profile percentages with all compounds.

Compound	CAS Number	Specie ID	E0	E10	E15
3,4-DIMETHYL-1-PENTENE	7385-78-6	209	0.000%	0.000%	0.000%
1-METHYLCYCLOPENTENE	693-89-0	103	0.036%	0.005%	0.000%
BENZENE	71-43-2	302	3.426%	3.793%	3.821%
CYCLOHEXANE	110-82-7	385	10.067%	5.622%	0.980%
2-METHYLHEXANE	591-76-4	194	0.068%	0.000%	0.571%
2,3-DIMETHYLPENTANE	565-59-3	140	0.269%	0.547%	0.000%
1,1-DIMETHYLCYCLOPENTANE	1638-26-2	20	0.000%	0.011%	0.000%
CYCLOHEXENE	110-83-8	388	0.269%	0.214%	0.009%
3-METHYLHEXANE	589-34-4	245	0.116%	0.254%	0.352%
CIS-1,3-DIMETHYLCYCLOPENTANE	2532-58-3	353	0.000%	0.018%	0.079%
3-ETHYLPENTANE	617-78-7	229	0.000%	0.024%	0.059%
TRANS-1,2-DIMETHYLCYCLOPENTANE	822-50-4	725	0.000%	0.006%	0.073%
TRANS-1,3-DIMETHYLCYCLOPENTANE	1759-58-6	727	0.000%	0.000%	0.000%
1-HEPTENE	592-76-7	76	0.000%	0.000%	0.000%
2,2,4-TRIMETHYLPENTANE	540-84-1	118	3.188%	1.227%	1.763%
HEPTANE	142-82-5	600	0.041%	0.293%	0.883%
UNIDENTIFIED C7	#N/A	2005	0.044%	0.000%	0.000%
2,4,4-TRIMETHYL-1-PENTENE	107-39-1	141	0.000%	0.332%	0.602%
2,3-DIMETHYL-2-PENTENE	10574-37-5	135	0.000%	0.000%	0.000%
METHYLCYCLOHEXANE	108-87-2	550	0.000%	0.476%	1.403%
2,2-DIMETHYLHEXANE	590-73-8	124	0.000%	0.000%	0.000%
1,1,3-TRIMETHYLCYCLOPENTANE	4516-69-2	13	0.000%	0.000%	0.065%
2,4,4-TRIMETHYL-2-PENTENE	107-40-4	142	0.000%	0.127%	0.201%
2,2,3-TRIMETHYLPENTANE	564-02-3	113	0.575%	0.184%	0.352%
2,4-DIMETHYLHEXANE	589-43-5	149	0.395%	0.183%	0.319%
1-TRANS-2-CIS-4-TRIMETHYLCYCLOPENTANE	#N/A	1540	0.000%	0.000%	0.039%
3,3-DIMETHYLHEXANE	563-16-6	206	0.000%	0.000%	0.000%
1-TRANS-2-CIS-3-TRIMETHYLCYCLOPENTANE	19374-46-0	1537	0.000%	0.000%	0.006%
2,3,4-TRIMETHYLPENTANE	565-75-3	130	1.084%	0.352%	0.497%
2,3,3-TRIMETHYLPENTANE	560-21-4	128	1.008%	0.349%	0.598%
TOLUENE	108-88-3	717	7.542%	7.440%	5.831%
2,3-DIMETHYLHEXANE	584-94-1	138	0.038%	0.056%	0.121%
2-METHYLHEPTANE	592-27-8	193	0.000%	0.135%	0.444%
3,4-DIMETHYLHEXANE	583-48-2	212	0.016%	0.000%	0.018%
4-METHYLHEPTANE	589-53-7	264	0.000%	0.004%	0.000%
3-METHYLHEPTANE	589-81-1	244	0.000%	0.102%	0.296%
1-CIS,2-TRANS,3-TRIMETHYLCYCLOPENTANE	#N/A	357	0.000%	0.067%	0.299%
TRANS-1,4-DIMETHYLCYCLOHEXANE	2207-04-7	729	0.000%	0.018%	0.111%
3-ETHYLHEXANE	619-99-8	226	0.000%	0.027%	0.000%
2,2,5-TRIMETHYLHEXANE	3522-94-9	121	0.495%	0.180%	0.283%
CIS-1-METHYL-3-ETHYLCYCLOPENTANE	#N/A	364	0.000%	0.000%	0.000%
TRANS-1,2-DIMETHYLCYCLOHEXANE	6876-23-9	724	0.000%	0.024%	0.130%
OCTANE	00111-65-9	604	0.000%	0.243%	0.788%
TRANS-2-OCTENE	13389-42-9	741	0.000%	0.000%	0.072%
2,3,5-TRIMETHYLHEXANE	1069-53-0	132	0.048%	0.000%	0.016%

Table 5 (cont.): Composite profile percentages with all compounds.

Compound	CAS Number	Specie ID	E0	E10	E15
2,4-DIMETHYLHEPTANE	2213-23-2	148	0.187%	0.019%	0.074%
CIS-1,2-DIMETHYLCYCLOHEXANE	2207-01-4	351	0.000%	0.033%	0.065%
ETHYLCYCLOHEXANE	1678-91-7	450	0.013%	0.078%	0.278%
2,6-DIMETHYLHEPTANE	1072-05-5	160	0.000%	0.000%	0.000%
2,5-DIMETHYLHEPTANE	2216-30-0	155	0.000%	0.018%	0.098%
3,3-DIMETHYLHEPTANE	4032-86-4	205	0.000%	0.000%	0.000%
3,5-DIMETHYLHEPTANE	926-82-9	215	0.000%	0.018%	0.098%
ETHYLBENZENE	100-41-4	449	1.683%	1.660%	1.258%
2,3-DIMETHYLHEPTANE	3074-71-3	137	0.006%	0.000%	0.013%
m- & p-XYLENE	1330-20-7	507	4.407%	4.347%	4.570%
2-METHYLOCTANE	3221-61-2	198	0.081%	0.093%	0.362%
3-METHYLOCTANE	2216-33-3	247	0.049%	0.040%	0.207%
STYRENE	100-42-5	698	0.085%	0.083%	0.368%
o-XYLENE	95-47-6	620	1.720%	1.697%	0.966%
1-NONENE	124-11-8	106	0.063%	0.018%	0.095%
TRANS-3-NONENE	20063-92-7	745	0.020%	0.000%	0.000%
NONANE	111-84-2	603	0.283%	0.144%	0.557%
ISOPROPYLBENZENE (CUMENE)	98-82-8	514	0.125%	0.123%	0.067%
2,2-DIMETHYLOCTANE	15869-87-1	125	0.046%	0.154%	0.106%
2,4-DIMETHYLOCTANE	4032-94-4	151	0.040%	0.099%	0.052%
n-PROPYLBENZENE	103-65-1	608	0.406%	0.401%	0.219%
1-METHYL-3-ETHYLBENZENE	620-14-4	89	1.367%	1.348%	1.156%
1-METHYL-4-ETHYLBENZENE	622-96-8	94	0.616%	0.608%	0.545%
1,3,5-TRIMETHYLBENZENE	108-67-8	44	0.629%	0.621%	0.506%
1-METHYL-2-ETHYLBENZENE	611-14-3	80	0.518%	0.511%	0.505%
1,2,4-TRIMETHYLBENZENE	95-63-6	30	1.159%	1.144%	1.319%
1-DECENE	872-05-9	996	0.000%	0.000%	0.000%
DECANE	124-18-5	598	0.000%	0.085%	0.130%
ISOBUTYLBENZENE	538-93-2	3	0.039%	0.039%	0.119%
METHYLPROPYLBENZENE (sec butylbenzene)	68411-44-9	499	0.000%	0.000%	0.058%
1-METHYL-3-ISOPROPYLBENZENE	535-77-3	90	0.058%	0.057%	0.000%
1,2,3-TRIMETHYLBENZENE	526-73-8	25	0.208%	0.205%	0.472%
1-METHYL-4-ISOPROPYLBENZENE	99-87-6	97	0.018%	0.018%	0.000%
INDAN	496-11-7	485	0.099%	0.110%	0.000%
1-METHYL-2-ISOPROPYLBENZENE	527-84-4	81	0.016%	0.015%	0.067%
1,3-DIETHYLBENZENE	141-93-5	51	0.286%	0.283%	0.018%
1,4-DIETHYLBENZENE	105-05-5	59	0.068%	0.067%	0.000%
1-METHYL-3-N-PROPYLBENZENE	1074-43-7	92	0.000%	0.000%	0.014%
1-METHYL-4-N-PROPYLBENZENE	1074-55-1	100	0.000%	0.000%	0.000%
1,2 DIETHYLBENZENE	135-01-3	36	0.053%	0.052%	0.064%
1-METHYL-2-N-PROPYLBENZENE	1074-17-5	84	0.000%	0.000%	0.037%
1,4-DIMETHYL-2-ETHYLBENZENE	1758-88-9	60	0.000%	0.000%	0.000%
1,3-DIMETHYL-4-ETHYLBENZENE	874-41-9	53	0.000%	0.000%	0.000%
1,2-DIMETHYL-4-ETHYLBENZENE	934-80-5	39	0.000%	0.000%	0.021%
1,3-DIMETHYL-2-ETHYLBENZENE	2870-04-4	52	0.000%	0.000%	0.000%

Table 5 (cont.): Composite profile percentages with all compounds.

Compound	CAS Number	Specie ID	E0	E10	E15
UNDECANE	1120-21-4	610	0.000%	0.009%	0.000%
1,2,4,5-TETRAMETHYLBENZENE	95-93-2	28	0.118%	0.117%	0.000%
2-METHYLBUTYLBENZENE (sec AMYLBENZENE)	538-68-1	83	0.000%	0.000%	0.000%
3,4 DIMETHYLCUMENE	#N/A	54	0.000%	0.000%	0.000%
1,2,3,5-TETRAMETHYLBENZENE	527-53-7	23	0.155%	0.153%	0.000%
TERT-1-BUT-2-METHYLBENZENE	#N/A	1655	0.000%	0.000%	0.000%
1,2,3,4-TETRAMETHYLBENZENE	488-23-3	22	0.095%	0.094%	0.000%
N-PENT-BENZENE	#N/A	606	0.000%	0.000%	0.000%
TERT-1-BUT-3,5-DIMETHYLBENZENE	#N/A	86	0.000%	0.000%	0.000%
NAPHTHALENE	91-20-3	611	0.033%	0.033%	0.000%
DODECANE	112-40-3	599	0.000%	0.000%	0.000%
1,3,5-TRIETHYLBENZENE	102-25-0	43	0.000%	0.000%	0.000%
UNIDENTIFIED C9-C12+	#N/A	327	0.272%	2.181%	1.331%
FORMALDEHYDE	50-00-0	465	0.927%	0.874%	1.072%
ACETALDEHYDE	75-07-0	279	0.453%	1.610%	2.232%
ACROLEIN	107-02-8	283	0.094%	0.072%	0.083%
ACETONE	67-64-1	281	0.419%	0.346%	0.498%
PROPIONALDEHYDE	123-38-6	673	0.122%	0.054%	0.048%
CROTONALDEHYDE	4170-30-3	382	0.026%	0.000%	0.000%
ISOBUTYRALDEHYDE	78-84-2	2119	0.010%	0.014%	0.011%
MEK	78-93-3	536	0.010%	0.014%	0.011%
BENZALDEHYDE	100-52-7	301	0.253%	0.168%	0.113%
ISOVALERALDEHYDE	590-86-3	517	0.060%	0.000%	0.000%
VALERALDEHYDE	110-62-3	845	0.102%	0.045%	0.038%
O-TOLUALDEHYDE	529-20-4	1467	0.040%	0.022%	0.034%
M/P-TOLUALDEHYDE	#N/A	2164	0.055%	0.043%	0.052%
HEXANALDEHYDE	#N/A	840	0.058%	0.037%	0.018%
DIMETHYLBENZALDEHYDE	#N/A	1712	0.019%	0.004%	0.050%
METHANOL	67-56-1	531	1.405%	0.536%	0.000%
ETHANOL	64-17-5	442	0.498%	3.806%	4.951%
2-PROPANOL	67-63-0	513	1.009%	0.637%	0.000%

Appendix A: SPECIATE4 IDs from Spec4Asn-8-10-06.xls

SPECIATE4 IDs from Spec4Asn-8-10-06.xls

Assignments for SPECIATE 4.0 081005R1.mdb. Rec'd from David Holoman 8/10/05.
Version with unknowns represented by REPUNK-1 and unassigned compounds represented by
REPNOA-1 mixtures Copied from EmitDB.XLS Master List assignments on 8/10/06

Specie ID	NAME	Specie ID	NAME
1	(1-Methylpropyl)benzene	61	1,4-dioxane
2	(2-methylbutyl)cyclohexane	62	1,4-isodipropylbenzene
3	(2-methylpropyl)benzene	63	1-(1,1-dimethylethyl)-3,5-dimethylbenzene
4	1,1,1-trichloroethane	64	1-butene
5	1,1,2,2-tetrachloroethane	65	1-butyne
6	1,1,2,3-tetramethylcyclohexane	66	1-decene, dimer, hydrogenated
7	1,1,2-trichloroethane	67	1-ethyl-1,2-dimethylcyclohexane
8	1,1,2-trimethylcyclohexane	68	1-ethyl-2,2,6-trimethylcyclohexane
9	1,1,2-trimethylcyclopentane	69	1-ethyl-2,4-dimethylcyclohexane
10	1,1,3,4-tetramethylcyclohexane	70	1-ethyl-2-methylcyclopentane
11	1,1,3,5-tetramethylcyclohexane	71	1-ethyl-2-npropylbenzene
12	1,1,3-trimethylcyclohexane	73	1-ethyl-3-methylcyclopentane
13	1,1,3-trimethylcyclopentane	74	1-ethyl-4-isopropylbenzene
14	1,1,4-trimethylcyclohexane	75	1-ethyltertbutylether
15	1,1-dichloro-1-fluoroethane	76	1-heptene
16	1,1-dichloroethane	77	1-hexanol
17	1,1-dichloroethene (vinylidene chloride)	78	1-hexene
18	1,1-dimethyl-2-propylcyclohexane	79	1-Methyl-1-ethylcyclohexane
19	1,1-dimethylcyclohexane	80	1-Methyl-2-ethylbenzene
20	1,1-dimethylcyclopentane	81	1-Methyl-2-isopropylbenzene
21	1,1-Methylethylcyclopentane	82	1-Methyl-2-isopropylcyclohexane
22	1,2,3,4-tetramethylbenzene	83	1-Methyl-2-n-butylbenzene
23	1,2,3,5-tetramethylbenzene	84	1-Methyl-2-npropylbenzene
24	1,2,3-trimethyl-4-ethylbenzene	85	1-Methyl-2-pyrrolidinone
25	1,2,3-trimethylbenzene	86	1-Methyl-2-tert-butylbenzene
26	1,2,3-trimethylcyclohexane	88	1-Methyl-3-butylbenzene
27	1,2,3-trimethylcyclopentane	89	1-Methyl-3-ethylbenzene
28	1,2,4,5-tetramethylbenzene	90	1-Methyl-3-isopropylbenzene
29	1,2,4-triethylbenzene	91	1-Methyl-3-isopropylcyclohexane
30	1,2,4-trimethylbenzene (1,3,4-trimethylbenzene)	92	1-Methyl-3-npropylbenzene
31	1,2,4-trimethylcyclopentane	94	1-Methyl-4-ethylbenzene
32	1,2,4-trimethylcyclohexane	95	1-Methyl-4-ethylcyclohexane
33	1,2-butadiene (methylallene)	96	1-Methyl-4-isobutylbenzene
34	1,2-dichloropropane	97	1-Methyl-4-isopropylbenzene
35	1,2-diethyl-1-methylcyclohexane	98	1-Methyl-4-isopropylcyclohexane
36	1,2-diethylbenzene (ortho)	99	1-methyl-4-n-pentylbenzene
37	1,2-dimethyl-3-ethylbenzene	100	1-Methyl-4-npropylbenzene
38	1,2-dimethyl-3-ethylcyclohexane	101	1-Methyl-4-t-butylbenzene
39	1,2-dimethyl-4-ethylbenzene	103	1-Methylcyclopentene
40	1,2-dimethylcyclopentane	104	1-Methylindan
41	1,2-epoxybutane	105	1-Methylnaphthalene
42	1,2-propadiene	106	1-nonene
43	1,3,5-triethylbenzene	107	1-octene
44	1,3,5-trimethylbenzene	108	1-pentene
45	1,3,5-trimethylcyclohexane	109	1-propyne
46	1,3-butadiene	110	2,2,3,3-tetramethylpentane
47	1,3-butadiyne	111	2,2,3,trimethylhexane
48	1,3-cyclopentadiene	112	2,2,3-trimethylbutane
49	1,3-dichlorobenzene (m-dichlorobenzene)	113	2,2,3-trimethylpentane
50	1,3-dichloropropene	114	2,2,4,6,6-pentamethylheptane
51	1,3-diethylbenzene (meta)	115	2,2,4-trimethyl-1,3-pentanediol isobutyrate (texanol)
52	1,3-dimethyl-2-ethylbenzene	116	2,2,4-trimethylheptane
53	1,3-dimethyl-4-ethylbenzene	117	2,2,4-trimethylhexane
54	1,3-dimethyl-4-isopropylbenzene	118	2,2,4-trimethylpentane
55	1,3-dimethyl-5-ethylbenzene	120	2,2,5-trimethylheptane
56	1,3-dioxolane	121	2,2,5-trimethylhexane
57	1,3-dipropylbenzene	122	2,2-dimethylbutane
58	1,3-n-dipropylbenzene	123	2,2-dimethylheptane
59	1,4-diethylbenzene (para)	124	2,2-dimethylhexane
60	1,4-dimethyl-2-ethylbenzene	125	2,2-dimethyloctane

Specie ID	NAME
126	2,2-dimethylpentane
127	2,2-dimethylpropane
128	2,3,3-trimethylpentane
129	2,3,4-trimethylhexane
130	2,3,4-trimethylpentane
131	2,3,5-trimethylheptane
132	2,3,5-trimethylhexane
133	2,3-dimethyl-1-butene
134	2,3-dimethyl-2-octene
135	2,3-dimethyl-2-pentene
136	2,3-dimethylbutane
137	2,3-dimethylheptane
138	2,3-dimethylhexane
139	2,3-dimethyloctane
140	2,3-dimethylpentane
141	2,4,4-trimethyl-1-pentene
142	2,4,4-trimethyl-2-pentene
143	2,4,4-trimethylhexane
144	2,4,5-trichlorophenol
145	2,4,5-trimethylheptane
146	2,4-dimethyl-1-pentene
147	2,4-dimethyl-2-pentene
148	2,4-dimethylheptane
149	2,4-dimethylhexane
150	2,4-dimethylnonane
151	2,4-dimethyloctane
152	2,4-dimethylpentane
153	2,4-pentanedione
154	2,4-toluene diisocyanate
155	2,5-dimethylheptane
156	2,5-dimethylhexane
157	2,5-dimethylnonane
158	2,5-dimethyloctane
159	2,6-dimethyldecane
160	2,6-dimethylheptane
161	2,6-dimethylnonane
162	2,6-dimethyloctane
163	2,6-dimethylundecane
164	2,7-dimethyldecane
165	2,7-dimethyloctane
166	2-(1-methylethoxy)phenol methylcarbamate (propoxur)
167	2-(2-butoxyethoxy)ethanol (butyl carbitol)
168	2-(2-ethylhexyloxy)ethanol
169	2-amino-2-methyl-1-propanol
170	2-butyne
171	2-chlorotoluene
172	2-ethoxyethanol (cellosolve) (egee)
173	2-ethoxyethyl acetate (cellosolve acetate)
174	2-ethyl hexyl acetate
175	2-ethyl-1,3-dimethylcyclohexane
176	2-ethyl-1-butene
177	2-hexenes
178	2-methoxy-1-propanol
179	2-methoxy-1-propanol acetate
180	2-methoxyethanol (methyl cellosolve) (egme)
181	2-methyl-1-butene
182	2-methyl-1-butyl acetate
183	2-methyl-1-octene
184	2-methyl-1-pentene
185	2-methyl-2-butene
186	2-methyl-2-hexene
187	2-methyl-2-pentene
188	2-methyl-2-propenal
189	2-methyl-3-ethylpentane
190	2-methyl-trans-3-hexene
191	2-methyldecalin
192	2-methyldecane
193	2-methylheptane
194	2-methylhexane

Specie ID	NAME
195	2-methylindan
196	2-methylnaphthalene
197	2-methylnonane
198	2-methyloctane
199	2-methylpentane
200	2-methylundecane (isododecane)
201	2-propenoic acid, 2-methyl dodecyl ester
202	3,3,5-trimethylheptane
203	3,3-dimethyl-1-butene
204	3,3-dimethyl-1-pentene
205	3,3-dimethylheptane
206	3,3-dimethylhexane
207	3,3-dimethyloctane
208	3,3-dimethylpentane
209	3,4-dimethyl-1-pentene
210	3,4-dimethyl-2-pentene
211	3,4-dimethylheptane
212	3,4-dimethylhexane
213	3,4-dimethyloctane
214	3,5-dimethyl-1-hexyne-3-ol
215	3,5-dimethylheptane
216	3,5-dimethylnonane
217	3,5-dimethyloctane
218	3,6-dimethyloctane
219	3,7-dimethylnonane
220	3-ethyl-2-methylheptane
221	3-ethyl-2-pentene
222	3-ethyl-3-methyloctane
223	3-ethyl-4-methylheptane
224	3-ethyldecane
225	3-ethylheptane
226	3-ethylhexane
227	3-ethylnonane
228	3-ethyloctane
229	3-ethylpentane
230	3-methyl-1-butene
231	3-methyl-1-hexene
232	3-methyl-1-pentene
233	3-methyl-3-ethylpentane
234	3-methyl-3-methoxy-1-butanol
235	3-methyl-cis-2-hexene
236	3-methyl-cis-2-pentene
237	3-methyl-cis-3-hexene
238	3-methyl-trans-2-hexene
239	3-methyl-trans-2-pentene
240	3-methyl-trans-3-hexene
242	3-methylcyclopentene
243	3-methyldecane
244	3-methylheptane
245	3-methylhexane
246	3-methylnonane
247	3-methyloctane
248	3-methylpentane
249	3-methylundecane
250	3-phenylpentane
251	4,4-dimethyl-2-neopentyl-1-pentene
252	4,4-dimethyl-2-pentene
253	4,4-dimethylheptane
254	4,5-dimethyldecane
255	4,5-dimethyloctane
256	4-ethyldecane
257	4-methyl-1-hexene
258	4-methyl-1-pentene
259	4-methyl-2-pentanol (methyl isobutyl carbinol)
260	4-methyl-cis-2-pentene
261	4-methyl-trans-2-hexene
262	4-methyl-trans-2-pentene
263	4-methyldecane
264	4-methylheptane
265	4-methylindan

Specie ID	NAME	Specie ID	NAME
266	4-methylnonane	349	Cis,trans-1,2,3-trimethylcyclohexane
267	4-methyloctane	350	Cis,trans-1,2,4-trimethylcyclohexane
268	4-methylundecane	351	Cis-1,2-dimethylcyclohexane
269	5-isopropylnonane	352	Cis-1,3-dimethylcyclohexane
270	5-methyl-1-hexene	353	Cis-1,3-dimethylcyclopentane
271	5-methyl-cis-2-hexene	354	Cis-1,4-dimethylcyclohexane
272	5-methyldecane	355	Cis-1,cis-2,3-trimethylcyclopentane
273	5-methylindan	356	Cis-1,cis-3,5-trimethylcyclohexane
274	5-methylnonane	357	Cis-1,trans-2,3-trimethylcyclopentane
275	5-methylundecane	358	Cis-1,trans-2,4-trimethylcyclopentane
276	6-ethyl-2-methyloctane	359	Cis-1,trans-2,trans-4-trimethylcyclohexane
277	6-methylundecane	360	Cis-1-2-dimethylcyclopentane
279	Acetaldehyde	361	Cis-1-ethyl-2-methylcyclohexane
280	Acetic acid	362	Cis-1-ethyl-2-methylcyclopentane
281	Acetone	363	Cis-1-ethyl-3-methylcyclohexane
282	Acetylene	364	Cis-1-ethyl-3-methylcyclopentane
283	Acrolein (2-propenal)	365	Cis-1-ethyl-4-methylcyclohexane
284	Acrylamide	367	Cis-2-butene
285	Acrylonitrile	368	Cis-2-heptene
286	Aggregate ingredients	369	Cis-2-hexene
287	Aggregated VOCs	370	Cis-2-octene
288	Aggregated exempt compounds	371	Cis-2-pentene
289	Aliphatic solvent	372	Cis-3-hexene
290	Aliphatics	373	Cis-3-nonene
291	Alkene ketone	374	Cis-bicyclo[3.3.0]octane
293	Amines, polyethylene poly compounds w/succinic	375	Cis-bicyclo[4.3.0]nonane
295	Amyl acetate	376	Cis-decalin
297	Aromatic 200 solvent	377	Citrus lemon peel oil
299	B-methylstyrene	378	Citrus terpene
301	Benzaldehyde	381	Cresylic acid (mixed cresols)
302	Benzene	382	Crotonaldehyde
303	Benzene derivatives	383	Cumene hydroperoxide
304	Benzothiazole	384	Cyclohexamine
305	Benzoyl peroxide	385	Cyclohexane
306	Benzyl alcohol	386	Cyclohexanol
308	Bromodichloromethane	387	Cyclohexanone
309	Butane, branched & linear	388	Cyclohexene
310	Butyl cellosolve (2-butoxyethanol) (egbe)	389	Cyclomethicone (a vms)
311	Butylbenzylphthalate	390	Cyclopentane
312	Butylcyclohexane	391	Cyclopentene
313	Butyraldehyde	392	D-limonene (4-isopropenyl-1-methylcyclohexane)
314	C10 alkylphenols	393	Decabromodiphenyl oxide
315	C10 aromatics	394	Di(2-ethylhexyl)phthalate
316	C10 internal alkenes	395	Di(propylene glycol) methyl ether
317	C11 alkylphenols	396	Diacetone
318	C11 dialkyl benzenes	398	Dibutyl phthalate
319	C11 internal alkenes	399	Dichlorobenzene (mixed isomers)
320	C12 dialkyl benzenes	400	Dichlorodifluoromethane
321	C12 internal alkenes	401	Dichloromethane (methylene chloride)
322	C3-c4 alkane propellant	402	Diethanolamine
323	C5 aldehyde	403	Diethyl aminoethanol
324	C6 aldehydes	404	Diethylamine
325	C8 cycloparaffins	405	Diethylcyclohexane
326	C9 aromatics	406	Diethylene glycol
327	C9-c12 isoalkanes	407	Diethylene glycol butyl ether acetate (2-2-(butoxyethoxy)ethyl acetate)
330	Camphor	408	Diethylmethylcyclohexanes
331	Carbitol (degee) (2-(2-ethoxyethoxy)ethanol)	409	Diglycidyl resorcinol ether (dgre)
332	Carbon disulfide	410	Dihydronaphthalene
333	Carbon tetrachloride	411	Diisobutyl ketone
335	Carbonyl sulfide	412	Diisopropyl adipate
336	Chlorafin	413	Diisopropylene glycol
338	Chlorinated paraffin	414	Dimethoate
340	Chlorobenzene	415	Dimethoxymethane
341	Chlorodifluoromethane	416	Dimethoxypropane
342	Chlorofluorohydrocarbons	417	Dimethyl ether
343	Chloroform	418	Dimethyl formamide
344	Chloropicrin	419	Dimethyl phthalate
345	Chlorothalonil	420	Dimethyl succinate
346	Chlorpyrifos	421	Dimethyl sulfide
348	Cis,cis-1,2,4-trimethylcyclohexane		

Specie ID	NAME	Specie ID	NAME
422	Dimethyl sulfoxide	495	Isobutylcyclohexane
423	Dimethylbenzylalcohol	496	Isobutylcyclopentane
424	Dimethylbutylcyclohexane	497	Isobutylene
425	Dimethylcyclopentane	498	Isocyanate
426	Dimethyldecane	499	Isomers of butylbenzene
427	Dimethylethylcyclohexane	500	Isomers of decane
428	Dimethylheptanes	501	Isomers of decyne
429	Dimethylnonane	502	Isomers of diethylbenzene
430	Dimethylundecane	503	Isomers of dodecane
431	Dimethyloctyne diol	504	Isomers of tridecane
432	Dipropylene glycol	505	Isomers of undecane
433	Dipropylene glycol dimethyl ether (mixed isomers)	506	Isomers of undecyne
434	Mineral spirits	507	Isomers of xylene
435	DL-limonene (dipentene)	508	Isopentane
437	Eptc (s-ethyl dipropylthiocarbamate)	509	Isophorone diamine
438	Ethane	510	Isophorone (3,5,5-trimethyl-2-cyclohexenone)
439	Ethanolamine	511	Isoprene
440	Ethyl acetate	512	Isopropyl acetate
441	Ethyl acrylate	513	Isopropyl alcohol
442	Ethyl alcohol	514	Isopropylbenzene (cumene)
443	Ethyl chloride	515	Isopropylcyclohexane
444	Ethyl cyanoacrylate	516	Isopropylmethylcyclohexane
445	Ethyl ether	517	Isovaleraldehyde
446	Ethyl mercaptan	518	Kerosene
447	Ethyl propylcyclohexanes	521	Lemon oil
448	Ethyl-3-ethoxypropionate	522	M & p-xylene
449	Ethylbenzene	523	M-cresol (3-methyl-benzenol)
450	Ethylcyclohexane	524	M-xylene
451	Ethylcyclopentane	527	Menthol
452	Ethylene	529	Methane
453	Ethylene dibromide	530	Methoxypropanol acetate
454	Ethylene dichloride		(straight; possibly used for pgmea)
455	Ethylene glycol	531	Methyl alcohol
456	Ethylene glycol butyl ether acetate	532	Methyl amyl ketone
	(2-butoxyethyl acetate)	533	Methyl bromide
457	Ethylene glycol methyl ether acetate	534	Methyl carbitol (2-(2-methoxyethoxy)ethanol) (degme)
	(methyl cellosolve acetate)	535	Methyl chloride
458	Ethylene glycol propyl ether (2-propoxyethanol)	536	Methyl ethyl ketone (2-butanone)
459	Ethylene oxide	537	Methyl ethyl ketoxime
461	Ethylmethylcyclohexanes	538	Methyl hexane
462	Ethylmethylhexane	539	Methyl isobutyl ketone
463	Ethyloctane	540	Methyl mercaptan
464	Ethyltoluenes (methylethylbenzenes)	541	Methyl methacrylate
465	Formaldehyde	542	Methyl n-butyl ketone
466	Formic acid	543	Methyl pentylcyclohexane
467	Fragrances	544	Methyl propyl ketone (2-pentanone)
469	Gamma- butyrolactone	545	Methyl propylcyclohexanes
470	Glutaraldehyde (a dialdehyde)	546	Methyl salicylate (an ester)
471	Glycerol	547	Methyl styrene (mixed) (vinyl toluene)
472	Glyceryl triacetate	548	Methyl t-butyl ether
473	Glycol ether dpnb	550	Methylcyclohexane
	(1-(2-butoxy-1-methylethoxy)-2-propanol)	551	Methylcyclopentane
474	Glycolic acid (hydroxyacetic acid)	552	Methyldecalins
475	Glycols	553	Methyldecene
476	Glyphosate, isopropylamine salt	554	Methylene(b)4-phenylisocyanate
478	HFC-152a		(methylene diphenyl diisocyanate)
479	Hexachlorobenzene	555	Methylenediphenylisocyanate polymeric
480	Hexylcyclohexane	556	Methylnaphthalenes
481	Hexylcyclopentane	557	Methyltri(ethylmethylketoxime) silane
482	Hexylene glycol (2-methyl-2,4-pentanediol)	558	Methyltrimethoxysilane
483	Hydrocarbon propellant (LPG, sweetened)	559	Methylvinylbis(n-methylacetamido) silane
484	Hydrocarbon propellant (LPG)	560	Mineral oil
485	Indane	561	Misc. acetates and esters (TOG portion)
486	Indene	562	Misc. acids
489	Isoamyl acetate	563	Misc. alcohols
490	Isobornyl acetate (2-camphanyl acetate)	564	Misc. alkyd, acrylic, and related resins (TOG portion)
491	Isobutane	565	Misc. amines
492	Isobutyl acetate	566	Misc. asphalt mixtures (TOG portion)
493	Isobutyl alcohol	567	Misc. copolymers, surfactants, resins (TOG portion)
494	Isobutyl isobutyrate	568	Misc. esters

Specie ID	NAME
569	Misc. ethyleneamines
570	Misc. glycol ethers and acetates
571	Misc. glycols, glycol ethers, and acetates
572	Misc. hydrocarbon propellants
573	Misc. hydrocarbon resins (TOG portion)
574	Misc. lvp VOC distillates
575	Misc. oils - linseed/tung/soy/etc. (TOG portion)
576	Misc. oxygenated compounds
577	Misc. proprietary VOC
578	Misc. silanes
579	Misc. styrene-containing material (TOG portion)
580	Misc. trimethylbenzenes
581	Misc. urethane-containing material (TOG portion)
582	Misc. vinyl/acrylic and other copolymers (TOG portion)
583	Misc./other VOC
584	Methyl isothiocyanate
585	Molinate
587	Monoisopropanolamine (1-amino-2-propanol)
588	Monoterpenes
589	Morpholine
590	N,n-dimethylethanolamine
591	N-(trichloromethylthio)phthalimide (folpet)
592	N-butane
593	N-butyl acetate
594	N-butyl acrylate
595	N-butyl alcohol
596	N-butylbenzene
597	N-butylcyclopentane
598	N-decane
599	N-dodecane
600	N-heptane
601	N-hexane
602	N-hexylbenzene
603	N-nonane
604	N-octane
605	N-pentane
606	N-pentylbenzene
607	N-propyl alcohol
608	N-propylbenzene
609	N-tridecane
610	N-undecane
611	Naphthalene
614	Nitromethane
616	Nonadiene
617	Nonylphenoxypoly(ethyleneoxy)ethanol (tergitol np-33) (triton(r) n-101)
618	O-cresol (2-methyl-benzenol)
619	O-dichlorobenzene
620	O-xylene
621	Octahydroindenes
622	Octahydropentalene
623	Octanol
624	Orange oil
625	Orange terpenes
627	Oryzalin
628	Other C10
629	Other C11
630	Other C12
631	Other C13
632	Other C14
633	Other C7
634	Other C8
635	Other C9
636	Other exempt propellants
637	Other glycol ethers
638	Other, lumped VOCs, individually < 2% of category
639	Other, lumped exempts, individually < 2% of category
640	Other, misc. VOC
641	Other, misc. VOC compounds aggregated in profile

Specie ID	NAME
642	Other, misc. exempt compounds aggregated in profile
643	Oxo-hexyl acetate
644	Oxydemeton-methyl
645	Oxyfluorfen
646	P-cresol (4-methyl-benzenol)
647	P-dichlorobenzene
648	P-xylene
650	Panthenol
651	Par
652	Parachlorobenzotrifluoride
653	Pebulate
654	Pendimethalin
655	Pentamethylbenzene
656	Pentanedioic acid, dimethyl ester
657	Pentylcyclohexane
658	Pentylcyclopentane
659	Pentylindenecyclohexane
660	Peracetic acid
661	Perchloroethylene
662	Perfluorocarbons c5/c6
663	Phenol (carbolic acid)
664	Phenoxyethanol
667	Pine oil
668	Polyethylene glycol 200
671	Propane
672	Propenylcyclohexane
673	Propionaldehyde
674	Propyl acetate
675	Propyl heptene
676	Propylcyclohexane
677	Propylcyclopentane
678	Propylene
679	Propylene carbonate
680	Propylene glycol
681	Propylene glycol butyl ether (1-butoxy-2-propanol)
682	Propylene glycol methyl ether (1-methoxy-2-propanol)
683	Propylene glycol monoethyl ether (1-ethoxy-2-propanol)
684	Propylene glycol monomethyl ether acetate (2-(1-methoxy)propyl acetate)
685	Propylene glycol n-propyl ether
686	Propylene glycol t-butyl ether (1-(1,1,-dimethylethoxy)-2-propanol)
687	Propylene oxide
688	Raw linseed oil
690	S-pentylbenzene
691	Santosol dimethyl ester
692	Sec-butyl alcohol
698	Styrene
701	T-amylmethylether
702	T-butyl acetate
703	T-butylbenzene
704	T-decahydronaphthalene
705	Terpene
706	Tert-butyl alcohol
707	Tetrahydrofuran
708	Tetrahydrofurfuryl alcohol
709	Tetramethylcyclopentane
710	Tetramethylpentanone
711	Tetramethylthiourea
713	Thiobencarb
716	Tolualdehyde
717	Toluene
718	Toluene diisocyanates (mixed isomers)
719	Total aggregate organic ingredients
720	Trans,cis-1,2,4-trimethylcyclohexane
721	Trans,trans-1,2,4-trimethylcyclohexane
722	Trans,trans-1,3,5-trimethylcyclohexane
723	Trans-1,2-dichloroethene
724	Trans-1,2-dimethylcyclohexane

Specie ID	NAME
725	Trans-1,2-dimethylcyclopentane
726	Trans-1,3-dimethylcyclohexane
727	Trans-1,3-dimethylcyclopentane
728	Trans-1,3-pentadiene
729	Trans-1,4-dimethylcyclohexane
730	Trans-1,cis-2,3-trimethylcyclopentane
732	Trans-1-ethyl-2-methylcyclohexane
733	Trans-1-ethyl-3-methylcyclohexane
734	Trans-1-ethyl-3-methylcyclopentane
736	Trans-1-methyl-3-ethylcyclopentane
737	Trans-2-butene
738	Trans-2-ethylmethylcyclopentane
739	Trans-2-heptene
740	Trans-2-hexene
741	Trans-2-octene
742	Trans-2-pentene
743	Trans-3-heptene
744	Trans-3-hexene
745	Trans-3-nonene
746	Trans-4-octene
747	Trichloroethylene
748	Trichlorofluoromethane
749	Trichlorotrifluoroethane-F113
750	Triethanolamine
751	Triethylamine
752	Triethylenetetramine
753	Trifluralin
754	Triisopropanolamine
755	Trimethylbenzenes (mixed)
756	Trimethylcyclohexane
757	Trimethylcyclohexanol
758	Trimethylcyclopentanone
759	Trimethylhexene
760	Trimethyloctanes
761	Turpentine
763	Unidentified nonfumigant active ingredients
766	Urethane prepolymer
768	Vinyl acetate
769	Vinyl chloride
770	Vinylacetylene
771	Vinyltrimethoxysilane
772	Voc ingredients
773	Volatile methyl siloxanes
774	Witch hazel
775	Xylene range solvent
776	Xylenol
839	Glyoxal
840	Hexaldehyde
845	Valeraldehyde
846	Acenaphthene
847	Acenaphthylene
849	Anthraquinone
852	Anthracene
854	Benz(a)anthracene
855	Benzo[a]pyrene BaP
857	Benzo[e]pyrene (BeP)
858	Benzo(ghi)perylene
859	Bibenzyl
860	Biphenyl
864	Benzo(c)phenanthrene
867	Chrysene
868	Coronene
873	Dibenzofuran , also noted as "DBZFUR"
877	1,2-dimethylnaphthalene
879	2,6&2,7-dimethylnaphthalene
880	1&2-ethylnaphthalene
881	9-fluorenone
882	Fluoranthene
883	Fluorene
884	Indeno[123-cd]pyrene

Specie ID	NAME
885	1-methylfluorene
886	1-methylphenanthrene
887	1-Methylpyrene
889	2-methylphenanthrene
890	3-methylbiphenyl
895	9-methylanthracene
898	1-phenylnaphthalene
901	Perylene
902	Phenanthrene
903	Perinaphthenone
904	Pyrene
905	Retene
908	2,3,5-trimethylnaphthalene
909	Xanthone
934	Acetovanillone-TMS , also noted as "acetva"
935	4-allyl-guaiacol-TMS , also noted as "a4gucl"
937	Benzoic acid-TMS
941	Decanoic acid-TMS
947	Guaiacol-TMS
950	Hexanoic acid-TMS
951	Hexanedioic acid-TMS
952	Isoeugenol-TMS , also noted as "isoeug"
954	Lauric acid-TMS
956	4-me-guaiacol-TMS , also noted as "m4gucl"
957	4-methyl-syringol-TMS , also noted as "m4syrg"
958	Myristic acid-TMS
959	Nonadecanoic acid-TMS
961	Palmitic acid-TMS
962	Pentadecanoic acid-TM
966	Stearic acid-TMS
967	Succinic acid-TMS
968	Syringaldehyde-TMS
969	Syringol-TMS , also noted as "syrgol"
970	Tridecanoic acid-TMS
976	Acetophenone
977	Beta-pinene
981	Butylbenzene
996	1-decene
997	Decanal
998	2-decanone
1001	1,2-dihydronaphthalene
1002	1,3-diisopropylbenzene
1003	1,4-diisopropylbenzene
1007	Dodecene
1013	2,3-benzofuran
1018	Heptanal
1020	Hexyl acetate
1028	5-isopropyl-m-xylene
1042	Eicosane
1043	Heptadecane
1045	Hexadecane
1047	Nonadecane
1048	Octadecane
1049	Pentadecane
1051	Tetradecane
1057	Nonanal
1065	Octanal
1079	1,2,3,4-tetrahydronaphthalene
1082	1-undecene
1083	Alpha-pinene
1093	1-butene + isobutene
1098	1,2,4-trimethylbenzene+t-butylbenzene
1118	1,3-hexadiene (trans)
1153	3-methyl-2-pentene
1165	Carbon monoxide
1167	2-Methylfluorene
1168	Methylphenanthrene
1169	Dimethylphenanthrenes
1170	Triphenylene
1171	Benzo[b]fluoranthene

Specie ID	NAME	Specie ID	NAME
1172	Benzo[ghi]fluoranthene	1531	c-Paraffin, C12
1173	Cyclopenta[cd]pyrene	1532	u-Paraffin, C13
1462	p-Tolualdehyde	1533	i-Paraffin, C12
1463	Biacetyl	1535	Cyclohexane, 1,2,4-trimethyl-
1464	Methylglyoxal	1536	Cyclopentane, 1-ethyl-3-methyl-, cis-
1465	1-Dodecene	1537	cis,trans,cis-1,2,3-trimethyl Cyclopentane
1466	1-Tridecene	1538	Cyclopentane, (1-methylethyl)-
1467	o-Tolualdehyde	1539	Hexane, 2,4-dimethyl
1468	2,5-Dimethylaldehyde	1540	Cis,trans,cis-1,2,4-trimethyl Cyclopentane
1469	2,2-Dimethyl-3-ethylpentane	1541	1,3-diethyl, trans cyclopentane
1470	Cyclohexane, 1-ethyl-4-methyl-, cis	1542	c-Paraffin, C7
1471	4-ethylheptane	1543	i-Paraffin, C7
1472	Cis,trans,cis-1,2,3-Trimethylcyclohexane	1544	c-Paraffin, C8
1473	Cyclohexane, 1-methyl-3-(1-methylethyl)-	1545	u-Paraffin, C8
1474	trans-1-methyl-3-propylcyclohexane	1546	4-Ethyl-octane
1475	Cis-1-methyl-3-propylcyclohexane	1547	p-xylene, 2-propyl-
1476	1-isopropyl-2-methylcyclohexane	1548	5-propyl-m-xylene
1477	Cyclohexane, 1,2,4-trimethyl-, (1a,2f,4a)-	1549	Cyclohexane, 2-ethyl-1,3-dimethyl
1478	1-ethyl-trans-3-methylcyclohexane	1550	4,5-dimethyl decane
1479	Bicyclo[3.3.1]nonane	1551	Cyclohexane, 1-methyl-2-propyl, trans
1480	Cis,cis,cis-1,2,3-trimethylcyclohexane	1552	3,5-dimethyl decane
1481	Pentane, 3,3-diethyl-	1553	c-Paraffin, C9
1482	trans octahydro Indene	1554	4-propyl-o-xylene
1484	Cyclohexane, 1-ethyl-2,3-dimethyl	1555	4-propyl-m-xylene
1485	Cyclohexane, 1,1,2,3-tetramethyl	1556	1,3-Diethyl-4-methylbenzene
1486	Cyclohexane, 1-methyl-4-propyl, trans	1557	4,7-dimethyl-2,3-dihydro-1-h-indenes
1487	Nonane, 3-ethyl	1558	3,5-Diethyltoluene
1488	Heptane, 2,3,4-trimethyl	1560	Unknown C10 Aromatics
1489	Cyclohexane, 1,2,3-trimethyl, cct	1561	Dimethyl indan
1490	1-methyl-2-propyl cyclopentane	1562	1-ethyl-2,4,5-trimethyl benzene
1491	Cyclohexane, 1,3-diethyl, cis	1563	toluene, 3,4-diethyl-
1492	4-ethyl Nonane	1564	1-ethyl-2,3,5-trimethyl benzene
1493	4,6-dimethyl decane	1565	2-ethyl-1,3,4-trimethyl benzene
1494	2,8-dimethyl decane	1566	Dimethyl, isopropyl benzene
1495	2,9-dimethyl decane	1567	Unknown C11 Aromatics
1496	1,2,3-trimethyl-5-ethyl benzene	1569	Ethyl isopropyl benzene
1497	2,7-dimethyl decane	1572	2-ethyl-mesitylene
1498	Cyclohexane, 1,2-diethyl, trans	1573	1,2-dimethyl-3-propyl benzene
1499	Cyclohexane, 1,3-diethyl, trans	1574	1,3-diethyl-2-methyl benzene
1500	Cyclohexane, 1-methyl-4-propyl, cis	1575	2-ethenyl-1,4-dimethyl benzene
1501	u-Paraffin, C10	1576	1,3-dimethyl-2-propyl benzene
1502	u-Paraffin, C9	1577	1,2-dimethyl-4-ethenyl benzene
1503	c-Paraffin, C10	1578	Cyclopentane, 1,2,4-trimethyl-, (1.alpha.,2.alpha.,4.beta.)-
1504	i-Paraffin, C10	1579	Cyclohexane, 1-ethyl-2,4-dimethyl
1505	i-Paraffin, C11	1580	Cyclohexane, 1-methyl-2-propyl, cis
1506	u-Paraffin, C11	1581	3-ethyl-1,2,4-trimethyl benzene
1507	u-Paraffin, C12	1582	Unknown C12 Aromatics
1508	c-Paraffin, C11	1583	4-ethyl decane
1509	2,3-Dimethyl decane	1584	1-Decene, 6-ethyl
1510	2,4-dimethyl decane	1585	1-Decene, 4-ethyl
1511	2,5-dimethyl decane	1586	trans-1-Ethyl-2-methyl-cyclopentane
1512	decahydro-2-methyl naphthalene	1587	2,6-Dimethyl-1-heptene
1513	2-methyl dodecane	1588	1,1,3,3-Tetramethylcyclopentane
1514	3-methyl dodecane	1589	Hexane, 3-ethyl-3-methyl-
1515	5-methyl dodecane	1590	Cis-1,1,3,4-tetramethylcyclopentane
1516	4-methyl dodecane	1591	1-Nonene, 7-methyl
1517	5-ethyl decane	1592	Bicyclo[3.2.1]octane
1518	3,6-dimethyl decane	1593	i-Paraffin, C9
1519	1-Decene, 8-ethyl	1594	Cis-1,2,trans-1,4-1,2,4-trimethylcyclohexane
1520	4,7-dimethyl decane	1595	N-heneicosane
1521	3,7-dimethyl decane	1596	N-docosane
1522	3,8-dimethyl decane	1597	n-Tricosane
1523	5-ethyl nonane	1598	n-Tetracosane
1524	i-Paraffin,C13	1599	n-Pentacosane
1525	Cyclohexane, 1,2-diethyl, cis	1600	N-hexacosane
1526	Undecane, 3-ethyl	1601	N-heptacosane
1527	Cyclohexane, 1,4-diethyl, trans	1602	Octacosane
1528	Undecane, 5-ethyl	1603	n-Nonacosane
1529	Cyclohexane, 1,4-diethyl, cis	1604	n-Triacontane
1530	Undecane, 2,6,10-trimethyl		

Specie ID	NAME	Specie ID	NAME
1605	N-hentriacontane	1678	5-ethyldihydro-2(3H)-furanone
1606	Dotriacontane	1679	5-propyldihydro-2(3H)-furanone
1607	n-Tritriacontane	1680	Nitrite
1608	n-Tettriacontane	1681	squalene
1609	Methylfluoranthene	1682	9-Hexadecenoic acid
1610	Benzo[k]fluoranthene	1683	9,12-Octadecadienoic acid
1611	1,8-Naphthalic anhydride	1684	5-heptyldihydro-2(3H)-furanone
1612	Methylguaicol	1685	5-octyldihydro-2(3H)-furanone
1613	Ethylguaicol	1686	5-nonyldihydro-2(3H)-furanone
1614	Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester	1687	5-decyldihydro-2(3H)-furanone
1615	Coniferaldehyde	1688	5-undecyldihydro-2(3H)-furanone
1616	propiovanillone	1689	5-dodecyldihydro-2(3H)-furanone
1617	Octanoic acid	1690	2,6,10-Trimethyldodecane
1618	Nonanoic acid	1691	norfarnesane
1619	Undecanoic acid	1692	2,6,10-trimethyltridecane
1620	Heptadecanoic acid	1693	norpristane
1621	pentacosanoic acid	1694	N-Nonylcyclohexane
1622	Hexacosanoic acid	1695	Cyclohexane, decyl-
1623	Octanedioic acid	1696	C2-fluorene
1624	Decanedioic acid	1697	3-methyl-phenanthrene
1625	Palmitoleic acid	1698	Anthracene, 2-methyl-
1626	Oleic acid	1699	9-methylphenanthrene
1628	Pimaric acid	1700	C2-MW 178 PAH
1629	Sandaracopimaric acid	1701	C3-MW 178 PAH
1630	Isopimaric acid	1702	Acephenanthrylene
1631	Benzocaine	1703	C1-MW 202 PAH
1632	sitostenone	1704	Pristane
1633	Guaicyl acetone	1705	Phytane
1634	Homovanillic Acid	1706	C3-naphthalenes
1635	Vanillin	1707	C4-naphthalenes
1636	Heptacosanoic acid	1708	N-Pentadecylcyclohexane
1637	Octacosanoic acid	1709	8B,13a-dimethyl-14B-n-butylpodocarpane
1638	Triacotanoic acid	1710	8B,13a-dimethyl-14B-[3'-methylbutyl]podocarpane
1639	nonacosanoic acid	1711	M- & p-tolualdehyde
1640	Alpha-Amyrin	1712	2,5-Dimethylbenzaldehyde
1641	Beta-Amyrin	1713	1-Indanone
1642	Glycerol Monopalmitate	1714	Dibenzothiophene
1643	Glycerol monooleate	1715	Dibenzothiazine
1644	1,2,3-Trimethoxybenzene	1716	Cyclohexane, undecyl-
1645	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	1717	Dodecylcyclohexane
1646	sinapinaldehyde	1718	tridecylcyclohexane
1647	n-Pentatriacotane	1719	N-tetradecylcyclohexane
1648	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	1720	C1-MW 228 PAH
1649	3-Ethylpentene	1721	C1-MW 226 PAH
1650	Danitol	1722	Benzo[j]fluoranthene
1651	2-Butene	1723	Indeno[1,2,3-cd]fluoranthene
1652	Methylindane	1724	22,29,30-trisnorneohopane
1654	Cis-2-Nonene	1725	17a(H),21B(H),29-norhopane
1655	t-1-Butyl-2-Methylbenzene	1726	17a(H),21B(H)-hopane
1656	2-Butanone, 3,3-dimethyl-	1727	Octadecanedioic acid
1658	Undecanal	1728	nonadecanedioic acid
1659	Dodecanal	1729	Methylbenzoic acid
1660	Tridecanal	1730	Hexadecylcyclohexane
1661	tetradecanal	1731	Heptadecylcyclohexane
1662	Pentadecanal	1732	octadecylcyclohexane
1663	Hexadecanal	1733	Cyclohexane, nonadecyl-
1664	Heptadecanal	1734	Eicosylcyclohexane
1665	2-Nonanone	1735	Heneicosylcyclohexane
1666	2-Undecanone	1736	20S-13B(H),17a(H)-diacholestane
1667	2-Tridecanone	1737	20R-13B(H),17a(H)-diacholestane
1668	2-Pentadecanone	1738	17a(H)-22,29,30-trisnorhopane
1669	2-tetradecanone	1739	22R&S,17a(H),21B(H)-30-homohopane
1670	Furfural	1740	22R&S,17a(H),21B(H)-30-bishomohopane
1671	trans-2-Decenal	1741	20R-5a(H),14B(H),17B(H)-cholestane
1672	2-undecenal	1742	20S-5a(H),14B(H),17B(H)-cholestane
1673	Heptanoic acid	1743	20R-5a(H),14a(H),17a(H)-cholestane
1674	Heptadecan-2-one	1744	20R&S-5a(H),14B(H),17B(H)-ergostane
1675	5-butyldihydro-2(3H)-furanone	1745	20R&S-5a(H),14B(H),17B(H)-sitostane
1676	5-pentyldihydro-2(3H)-furanone	1746	P-diethylbenzene & n-butylbenzene
1677	5-hexyldihydro-2(3H)-furanone	1747	2-methylfuraldehyde

Specie ID	NAME	Specie ID	NAME
1748	Hydroxymethylfurfural	1820	2-Furancarboxaldehyde, 5-(hydroxymethyl)-
1749	3,4-Dimethoxybenzoic acid	1821	Iso-nonacosane
1750	1,2-dimethoxy-4-methyl benzene	1822	Vitamin E
1751	2-oxobutanal	1823	Niacin
1752	Phenol, 2-methoxy-4-(1-propenyl)-, (E)- ; trans-isoeugenol	1824	Glyoxylic Acid
1753	Phenol, 2-methoxy-4-propyl-	1825	Pyruvic acid
1754	Phenol, 4-ethyl-2-methoxy-	1826	N-Oxynicotine
1755	1,2-Benzenediol	1827	Hydroxypyridine
1756	Hydroquinone	1828	Furancarboxylic acid
1757	Resorcinol	1829	Phenylacetic Acid
1758	4-hydroxy benzeneethanol	1830	anteiso-Triacontane
1759	1,6-Dimethylnaphthalene	1831	Iso-Hentriacontane
1760	Phenol, 2,6-dimethyl-	1832	anteiso-Dotriacontane
1762	Hydroxybenzaldehydes	1833	Iso-triacontane
1763	Guaiacyl acetone	1834	Ethenylbenzenediols
1764	4-ethylsyringol	1835	9,12,15-Octadecatrienoic acid
1765	4-propylsyringol	1836	2-(2-Butoxyethanoxy)ethanol
1766	allylsyringol	1837	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
1767	4-propenylsyringol	1838	2,2,4-Trimethyl-1,3-pentanediol monoisobutyrate
1768	syringyl acetone	1839	Beryllium
1770	Dibenzo[def,mno]chrysene; anthanthrene	1840	Heptylcyclohexane
1772	n-pentacosanoic acid	1841	Octylcyclohexane
1773	N-hexacosanoic acid	1843	Cyclohexane, tetradecyl-
1774	n-9-octadecenoic acid	1845	8B,13a-dimethyl-14B- [3'-methylbutyl]-podocarpane
1775	n-9,12-octadecadienoic acid	1846	18a(H)-22,29,30- trisnorneohopane
1776	8,15-pimaradien-18-oic acid	1847	Tellurium
1777	Benzaldehyde, 3,4-dimethoxy-	1848	Dibenz[a,h]anthracene
1778	propionylsyringol	1849	Dysprosium
1779	Butyrylsyringol	1850	Lithium
1780	sinapylaldehyde	1851	Neodymium
1781	n-tetracosanoic acid	1852	Niobium
1782	other sugars	1853	Praseodymium
1783	7-oxodehydroabietic acid	1854	Samarium
1784	abieta-6,8,11,13,15-pentaen-18-oic acid	1855	Scandium
1785	abieta-8,11,13,15-tetraen-18-oic acid	1856	Tantalum
1786	Dodecenal	1857	Terbium
1787	tridecenal	1858	Thorium
1788	Tetradecenal	1859	Tungsten
1789	pentadecenal	1860	Boron
1790	2-heptadecanone	1861	Cerium
1792	9,12-octadecadienoic acid (linoleic)	1862	Cesium
1793	9,12,15-octadecatrienoic acid (linolenic)	1863	Europium
1794	n-9-Hexadecenoic acid	1864	Gadolinium
1795	n-Triacontanoic acid	1865	Germanium
1796	n-Octacosanoic acid	1866	Hafnium
1797	N-heptacosanoic acid	1867	Holmium
1798	n-Nanadecanoic acid	1868	Ytterbium
1799	o-Pentadecanoic acid	1869	Bismuth
1800	Neophytadiene	1870	Iodine
1801	C2-Naphthalenes	1871	Fluorine
1802	C1-MW 178 PAH	1872	hydrogen phosphate
1803	Solanone	1873	Acridine
1804	Geranyl acetone	1874	BENZO(B)NAPTHOL(1,2
1805	Nicotine	1875	BENZO(B+K)FLUORANTHE
1806	Bipyridyl	1876	WAT. SOL. CHLORIDE
1807	Cotinine	1877	WAT. SOL. POTASSIUM
1808	Carbazole	1879	4-Methylcyclopentene
1809	Indole	1880	methylsyringol
1810	Normicotine	1881	2,6-Dimethylnaphthalene
1811	Phenylpyridine	1882	propylguaicol
1812	quinoline	1883	Methyl fluorene
1813	Isoquinoline	1884	PM Fine
1814	2-Ethylphenol	1885	1-ETHOXY-2-PROPANOL
1815	Ethenylphenol	1886	1-METHYLCYCLOHEXENE
1816	2,5-Pyrrolidinedione, 1-methyl-(N-Methylsuccinimide)	1887	1-NITROPROPANE
1817	Beta-Nicotyrine	1888	2,2 DICHLORONITROANILINE
1818	Methylindole	1889	2,3,3-TRIMETHYL-1-BUTENE
1819	pyrolo[2,3-b]pyridine	1890	2-BUTYLTETRAHYDROFURAN
		1891	2-ETHYL HEXANOL
		1892	2-METHYL-3-HEXANONE

Specie ID	NAME
1893	3-(CHLOROMETHYL)-HEPTANE
1894	3,4 DIMETHYLOCTANE
1895	3-HEPTENE
1896	4,4-METHYLENE DIANILINE
1897	4-CHLORO-3,5-XYLENOL
1898	4-METHYLANILINE
1899	4-PHENYL-1-BUTENE
1900	5-CHLORO-2-METHYL-4-ISOTHIAZOLIN-3-ONE
1901	ACETIC ANHYDRIDE
1902	ACETONITRILE
1903	ACRYLIC ACID
1904	ALPHA-TERPINEOL
1905	AMINOANTHRAQUINONE
1906	ANILINE
1907	BENZOPYRENES
1908	BENZYL ACETATE
1909	BENZYL CHLORIDE
1910	BENZYLAMINE HYDROCHLORIDE
1911	BENZYL CARBONYL PROPIONATE
1912	BIPHENYLOL
1913	BIS(TRI-N-BUTYL TIN)OXIDE
1914	B-PHELLANDRENE
1915	BROMODINITROANILINE
1916	BROMODINITROBENZENE
1917	BUTOXY PROPANOL
1918	BUTOXYBUTENE
1919	BUTYL
1920	BUTYL BENZOATE
1921	BUTYLISOPROPYLPHthalate
1922	C-1 COMPOUNDS
1923	C10 AROMATIC
1924	C-10 COMPOUNDS
1925	C10 OLEFINS
1926	C10 PARAFFINS
1927	C10H12
1928	C10H16
1929	C-11 COMPOUNDS
1930	C11 OLEFINS
1931	C-12 COMPOUNDS
1932	C12 OLEFINS
1933	C-13 COMPOUNDS
1934	C13-BRANCHED ALKANE
1935	C-14 COMPOUNDS
1936	C14-BRANCHED ALKANE
1937	C-15 COMPOUNDS
1938	C15-BRANCHED ALKANE
1939	C16 BRANCHED ALKANE
1940	C-16 COMPOUNDS
1941	C16-BRANCHED ALKANE
1942	C-17 COMPOUNDS
1943	C-18 COMPOUNDS
1944	C-19 COMPOUNDS
1945	C2 ALKYL INDAN
1946	C-2 COMPOUNDS
1947	C2 CYCLOHEXANE
1948	C-20 COMPOUNDS
1949	C-21 COMPOUNDS
1950	C-22 COMPOUNDS
1951	C-23 COMPOUNDS
1952	C-24 COMPOUNDS
1953	C-25 COMPOUNDS
1954	C-26 COMPOUNDS
1955	C-27 COMPOUNDS
1956	C-28 COMPOUNDS
1957	C-29 COMPOUNDS
1958	C2-ALKYL-ANTHRACENES
1959	C2-ALKYL-BENZANTHRACENES
1960	C2-ALKYLNAPHTHALENE
1961	C-2-OCTENE
1962	C-3 COMPOUNDS

Specie ID	NAME
1963	C3 CYCLOHEXANE
1964	C3/C4/C5 ALKYL BENZENES
1965	C-30 COMPOUNDS
1966	C-31 COMPOUNDS
1967	C-32 COMPOUNDS
1968	C-33 COMPOUNDS
1969	C-34 COMPOUNDS
1970	C-35 COMPOUNDS
1971	C-36 COMPOUNDS
1972	C-37 COMPOUNDS
1973	C-38 COMPOUNDS
1974	C-39 COMPOUNDS
1975	C-3-HEXENE
1976	C-4 COMPOUNDS
1977	C4 SUBSTITUTED CYCLOHEXANE
1978	C4 SUBSTITUTED CYCLOHEXANONE
1979	C-40 COMPOUNDS
1980	C-41 COMPOUNDS
1981	C-42 COMPOUNDS
1982	C-43 COMPOUNDS
1983	C4-ALKYLPHENOLS
1984	C4-ALKYLSTYRENES
1985	C4-BENZENE
1986	C-5 COMPOUNDS
1987	C5 CYCLOHEXANE
1988	C5 ESTER
1989	C5 OLEFIN
1990	C5 PARAFFIN
1991	C5 PARAFFIN/OLEFIN
1992	C5 SUBSTITUTED CYCLOHEXANE
1993	C5-ALKYLBENZENES
1994	C5-ALKYLBENZENES (UNSAT.)
1995	C5-ALKYLPHENOLS
1996	C5-BENZENE
1997	C5-CYCLOHEXANE
1998	C5-ENE
1999	C-6 COMPOUNDS
2000	C6 OLEFINS
2001	C6 SUBSTITUTED CYCLOHEXANE
2002	C6-ALKYLBENZENE
2003	C6H18O3SI3
2004	C6H8 ISOMER
2005	C-7 COMPOUNDS
2006	C-7 CYCLOPARAFFINS
2007	C7 OLEFINS
2008	C7 PARAFFINS
2009	C7-C16 PARAFFINS
2010	C7H12O
2011	C-8 COMPOUNDS
2012	C-8 CYCLOPARAFFINS
2013	C-8 OLEFINS
2014	C8 PARAFFIN
2015	C8 PHENOLS
2016	C8H14
2017	C8H24O4SI4
2018	C-9 COMPOUNDS
2019	C-9 CYCLOPARAFFINS
2020	C9 OLEFINS
2021	C9 PARAFFIN
2022	C9 PHENOLS
2023	CAMPHERE
2024	CARBARYL
2025	CARYOPHYLLENE
2026	CHLOROPENTAFLUOROETHANE
2027	CHLOROPRENE
2028	CHLOROTOLUENE
2029	CHLOROTRIFLUOROMETHANE
2030	CIS-1,3-DICHLOROPROPYLENE
2031	COAL TAR
2032	COPPER NAPHTHENE

Specie ID	NAME
2033	CORN OIL
2034	CREOSOTE
2036	CYCLOPENTYLCYCLOPENTANE
2037	DECALINS
2038	DECYL ALCOHOL
2039	DENATURANT
2040	DI(ETHYLPHENYL) ETHANE
2041	DIAZINON
2042	DIBENZANTHRACENES
2043	DIBENZOPYRENES
2044	DIBUTYL ETHER
2045	DI-C8 ALKYL PHTHALATE
2046	DICHLOROTETRAFLUORETHANE
2047	DIETHYL ACETAL ACETALDEHYDE
2048	DIGLYCOLAMINE
2049	DIHYDRONAPHTHALENE
2050	DIHYDROXYACETONE
2051	DIHYDROXYNAPHTHALENEDIONE
2052	DIISOPROPYL BENZENE
2053	DIMETHYL ALKYL AMINES
2054	DIMETHYL NAPHTHALENE
2055	DIMETHYL TEREPHTHALATE
2056	DIMETHYLACETAMIDE, N,N-
2057	DIMETHYLAMINE
2058	DIMETHYLBUTENE
2059	DIMETHYLCARBAMODITHIOIC ACID, POTASSIUM SALT
2061	DIMETHYLCYCLOHEXANE
2062	DIMETHYLCYCLOPENTENES
2063	DIMETHYLETHYLBENZOIC ACID
2064	DIMETHYLHEPTANOL
2065	DIMETHYLHEXADIENE
2066	DIMETHYLHEXANEDIOATE
2067	DIMETHYLHEXANES
2068	DIMETHYLHEXENE
2069	DIMETHYLINDANS
2070	DIMETHYLINDENE
2071	DIMETHYLNAPHTHYRIDINE
2072	DIMETHYLNONANES
2073	DIMETHYLOCTANES
2074	DIMETHYLOCTANOL
2075	DIMETHYLOCTYNE
2076	DIMETHYLPENTANE
2077	DIMETHYLPENTANOL
2078	DIMETHYLPENTENE
2079	DIPROPYL PHTHALATE
2080	DIPROPYLENE GLYCOL ETHYL ETHER
2081	DIVINYL BENZENE
2082	DODECANAMIDE
2083	EPICHLOROHYDRIN
2084	ETHYL STYRENE
2085	ETHYLAMINE
2086	ETHYLBICYCLOHEPTANE
2087	ETHYLCYCLOPENTENE
2088	ETHYLDIMETHYLBENZENE
2089	ETHYLDIMETHYLCYCLOHEXANE
2090	ETHYLDIMETHYLPENTANE
2091	ETHYLENEAMINES
2092	ETHYLENEDIAMINETETRAACETIC ACID
2093	ETHYLHEPTANE
2094	ETHYLHEPTENE
2095	ETHYLHEXANOATE
2096	ETHYLINDAN
2097	ETHYLISOPROPYL ETHER
2098	ETHYLMETHYLCYCLOPENTANE
2099	ETHYLMETHYLOCTANE
2100	ETHYLOCTENE
2101	ETHYLPENTENE
2102	ETHYL-PHENYL-PHENYL-ETHANE
2103	ETHYLPROPYLCYCLOHEXANES

Specie ID	NAME
2104	FREON
2105	FURFURYL ALCOHOL
2106	GERANIOL
2107	HEPTADIENAL
2108	HEPTENE
2109	HEXACHLOROETHANE
2110	HEXADIENAL
2111	HEXAFLUOROETHANE
2112	HEXAMETHYLCYCLOTIRISILOXANE
2113	HEXAMETHYLENEDIAMINE
2114	HEXENAL
2115	HEXENE
2116	HEXYNE
2117	ISOAMYL ALCOHOL
2118	ISOBUTYL ACRYLATE
2119	ISOBUTYRALDEHYDE
2120	ISOMERS OF BUTENE
2121	ISOMERS OF C10H18
2122	ISOMERS OF C11H20
2123	ISOMERS OF C9H16
2124	ISOMERS OF ETHYLTOLUENE
2125	ISOMERS OF HEPTADECANE
2126	ISOMERS OF HEPTANE
2127	ISOMERS OF HEXANE
2128	ISOMERS OF NONANE
2129	ISOMERS OF OCTADECANE
2130	ISOMERS OF OCTANE
2131	ISOMERS OF PENTADECANE
2132	ISOMERS OF PENTANE
2133	ISOMERS OF PENTENE
2134	ISOMERS OF PROPYLBENZENE
2135	ISOMERS OF TETRADECANE
2136	KEROSENE/DIESEL/FUEL OIL
2137	KETONES - GENERAL
2138	LACTOL SPIRITS
2139	MALATHION
2140	MALEIC ANHYDRIDE
2141	MEDIUM ALIPHATIC SOLVENT NAPHTHA
2142	MESITYL OXIDE
2143	METHOXYPROPANOL
2144	METHYL ACRYLATE
2145	METHYL BIPHENYL
2146	METHYL C11 ESTER
2148	METHYL C13 ESTER
2149	METHYL C14 ESTER
2150	METHYL C15 ESTER
2151	METHYL C19 ESTER
2152	METHYL C20 ESTER
2153	METHYL DODECANOATE
2154	METHYL FORMATE
2155	METHYL ISOAMYL KETONE
2157	METHYL NAPHTHALENES
2158	METHYL PALMITATE
2159	METHYL STEARATE
2160	METHYLACETATE
2161	METHYLLALLENE
2162	METHYLAMINE
2163	METHYL-ANTHRACENES
2164	METHYLBENZALDEHYDE
2165	METHYL-BENZANTHRACENES
2166	METHYLBUTADIENE
2167	METHYLBUTENE
2168	METHYLCYCLOHEXADIENE
2169	METHYLCYCLOHEXENE
2170	METHYLCYCLOOCTANE
2171	METHYLCYCLOPENTADIENE
2172	METHYLDECANES
2173	METHYLDIHYDRONAPHTHALENE
2174	METHYLDODECANE
2175	METHYLENE BROMIDE

Specie ID	NAME
2176	METHYLETHYLPENTANOATE
2177	METHYL-FLUORANTHENES
2178	METHYLHEPTANE
2179	METHYLHEPTANOL
2180	METHYLHEPTENE
2181	METHYLHEPTYNE
2182	METHYLHEXADIENE
2183	METHYLHEXANAL
2184	METHYLHEXANE
2185	METHYLHEXENES
2186	METHYLINDANS
2187	METHYLINDENE
2188	METHYLISOPROPYLCYCLOHEXANE
2189	METHYLMETHYLPROPENOATE
2190	METHYLNAPHTHALENE
2191	METHYLNONANE
2192	METHYLNONENE
2193	METHYLOCTANES
2194	METHYLPENTANE
2195	METHYLPENTENES
2196	METHYLPROPENE
2197	METHYLPROPYLCYCLOHEXANES
2198	METHYLPROPYLNONANE
2199	METHYLUDECANE
2200	M-XYLENE AND P-XYLENE
2201	MYRCENE
2202	N,N-DIETHYL-3-METHYLBENZAMIDE
2203	NAPHTHA
2204	NAPHTHENIC ACID
2205	NAPHTHOL
2206	NITROBENZENE
2207	NONENONE
2208	N-PENTENE
2209	N-PENTYLCYCLOHEXANE
2210	N-PHENYLANILINE
2211	OCTAMETHYLCYCLOTETRASILOXANE
2212	OCTATRIENE
2213	OTHER
2214	OXALIC ACID (ANHYDROUS)
2215	OXYGENATES
2216	PARAFFINS (C16-C34)
2217	PARAFFINS/OLEFINS (C12-C16)
2218	PARAFORMALDEHYDE
2219	PENTACHLORONITROBENZENE
2221	PENTANOL
2223	PENTYL ALCOHOL, TERT-
2224	PENTYLIDENECYCLOHEXANE
2225	PENTYNE
2226	PETROLEUM ETHER
2227	PHENYL ISOCYANATE
2228	PHTHALIC ANHYDRIDE
2229	PINE TAR
2230	PIPERYLENE
2231	PRAMITOL
2232	PREDNISONE
2233	PROPIONIC ACID
2234	PROPYLENE DICHLORIDE
2235	PROPYLENE GLYCOL PHENYL ETHER
2236	PROPYLHEPTENES
2237	PYRETHRUM
2238	PYRIDINE
2239	SILICONE
2240	SILOXANE
2241	STODDARD SOLVENT
2242	SUBSTITUTED C9 ESTER (C12)
2243	T-1-PHENYLBUTENE
2244	T-2-NONENE
2245	TENNECO 500-100
2246	TEREPHTHALIC ACID
2247	TERPENE ALCOHOL

Specie ID	NAME
2248	TERPENES
2249	TETRABUTYL ORTHOTITANATE
2250	TETRACHLOROBENZENES
2251	TETRAETHYLENE GLYCOL
2252	TETRAFLUOROMETHANE
2253	TETRAMETHYLBENZENE
2254	TETRAMETHYLCYCLOBUTENE
2255	TETRAMETHYLHEXANE
2256	TOTAL AROMATIC AMINES
2257	TOTAL C2-C5 ALDEHYDES
2258	TRANS-1,3-DICHLOROPROPENE
2259	TRICHLOROBENZENES
2260	TRIETHANOLAMINE LAURYL SULFATE
2261	TRIETHYLENE GLYCOL
2262	TRIETHYLENE GLYCOL MONOBUTYL ETHER
2263	TRIFLUOROMETHANE
2264	TRIMETHYLAMINE
2265	TRIMETHYLDECANE
2266	TRIMETHYLDECENE
2267	TRIMETHYLFLUOROSILANE
2268	TRIMETHYLHEPTANES
2269	TRIMETHYLHEXANES
2270	TRIMETHYLINDAN
2271	TRIMETHYLPENTADIENE
2272	TRIMETHYLPENTANE
2273	UNC PEAKS TO CBM ALDEHYDES
2274	UNC PEAKS TO CBM NON REACT
2275	UNC PEAKS TO CBM OLEFINS
2276	UNC PEAKS TO CBM PARAFFINS
2277	UNC PEAKS TO CBM TOLUENE
2278	UNC PEAKS TO CBM XYLENE
2279	UNDEFINED AROMATIC
2280	UNDEFINED PARAFFIN
2281	UNDEFINED PETROLEUM DISTILLATES
2282	UNDEFINED PROPELLANT
2283	UNDEFINED VOC
2284	UNIDENTIFIED
2285	UNKNOWN #1
2286	UNKNOWN #13
2287	UNKNOWN #16
2288	UNKNOWN #3
2289	UNKNOWN #4
2290	UNKNOWN #5
2291	UNKNOWN #6
2292	UNKNOWN #7
2293	UNKNOWN #8
2294	VARAMID ML 1
2295	XYLENE BASE ACIDS
2297	Unknown
2300	Trimethylcyclopentane
2301	Dimethylbutane