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Improvement of Speciation Profiles for Architectural and Industrial Maintenance Coating Operations

CALIFORNIA ENVIRONMENTAL PROTECTION AGENCY
AIR RESOURCES BOARD
Research Division

IMPROVEMENT OF SPECIATION PROFILES FOR ARCHITECTURAL AND INDUSTRIAL MAINTENANCE COATING OPERATIONS

Final Report 93-319

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Abstract

In this study, the nature of emissions from architectural and industrial maintenance coatings was examined. Coating materials for investigation were arranged into 11 categories, based on similarity of emissions, carrier technology, and sales-weighted VOC values. Detailed species profiles were obtained for 106 samples of water-based and solvent-based coating samples.

Emission profiles were obtained by a number of direct and chamber methods. A distillation method was developed for removing the solvents from the coating samples for analysis. Species profiles were developed using a combination of GC-FID and GC-MS.

These individual profiles were arranged into composite group profiles. The resulting profiles contained as many as several hundred identified components. The overall identification rate of VOC species was high. For water based samples, 100% of the VOC mass was identified in all but four samples. In these cases, a few percent of unknown species were detected. For the solvent-based coatings, the identification rate was over 90%, even in the worst case. For those components not positively identified, a carbon number was assigned, based on the retention index of the peak.

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I. Introduction

A. Statement of the Problem

Due to its reactivity and role in the formation of photochemical smog, much attention has been directed to the control of tropospheric ozone in California. In recognition of the significance of the pollutant, the ambient standard for ozone in California is more stringent than the federal standard (0.09 vs. 0.12 PPM, hourly average). In 1992, 11 of the 14 air basins in California reported ozone concentrations in excess of the California Ambient Air Quality Standard[1]. The Air Resources Board has developed control strategies for ozone based on computer models which simulate the production of ozone within a given receptor grid. One such model, the Urban Airshed Model (UAM)[2], accounts for the ozone forming potential originating from a host of hydrocarbon emissions of varying reactivity. The model allows the impact of various control strategies to be observed. Accurate data on the chemical composition of each hydrocarbon source class is essential for proper model operation. These "organic gas species profiles" must be continuously updated to reflect changes in hydrocarbon use patterns within the state.

Emissions from architectural and all industrial coating operations constitute a sizable portion of the total daily non-methane organic gases (roughly, 400 out of 1800 tons per day[3]) in California. The compositions of industrial and architectural coatings have changed significantly in the last few years, following legislation designed to reduce the types and amounts of volatile organic compounds (VOC) emitted by these coatings. Thus, existing species profiles for this class of substances do not accurately reflect the coating formulations now in use in California. This fact has been noted in the literature[3].

This study was intended to upgrade the species profiles for a number of sources within the general categories of industrial and architectural coating operations. Data were collected, based on direct emission measurements during the drying period, and information on the chemical composition of the coatings themselves. Comparisons of calculation-based and direct emission measurements were made. Specific sources were combined to render meaningful, composite species profiles that represent the impact of painting and coating activities on California's air quality.

References

1. California Air Resources Board, Annual Summary of Air Quality Data, Vol. XXIV (1992)
2. Systems Applications International, Description of the Urban Airshed Model, February, 1993
3. Harley, Robert A., Michael Hannigan and Glen R. Cass, *Environ. Sci. Technol.*, 28(12), 2395-2408 (1992)

List of Tables

Sales and use patterns of coatings have remained fairly stable over the past decade, as the information in the following tables indicate. These data indicate that the coatings industry is a mature one, with small. consistent growth over the past decade.

Major Uses of Coatings

Coating Sales in U.S. (in millions)
1989: 1.04 billion gallons
1983: 924 million gallons

	1989	1983
Architectural	$4,990	$3990
Product Finishes	$4,666	$3000
Special Purpose Coatings	$2,680	$1700
Miscellaneous Products	$1,100	$ 300

Major Producers of Coatings
(U.S. sales, in $millions)

	1989	1990
Sherwin-Williams	2,123	2,267
Valspar	527	531
Grow Group	411	439
RPM-Ohio	396	412
Standard Brands	315	298
Lilly Industrial Coating	212	232
Guardsman	150	193

Over the past decade, there has been a steady decline in the amount of solvent used by the coating industry. The decline in solvent use by the coatings industry roughly parallels the overall decline in U.S.solvent use. The C&E News Report on Solvents projects a continuing gradual decline in solvent use on the order of 1.6% per year through 1997.

Solvent Use Patterns
(millions of pounds, in the U.S.)

	1987	1992
total solvents	16,341	12,571
solvents for coatings	10,081	6,826
% for coatings	62%	54%

While there are many constant factors in the economics of the paint and coatings industry, there has been a shift in coatings technology away from the "conventional" low-solids, solvent-based systems that were common in 1980 to systems with high solids, and increased reliance on water-based systems.

These data suggest that use patterns and volumes of coatings materials will remain near the current levels for some time. It also adds credibility to using the results of a 1990 ARB Survey as a starting point for identifying related groups of coatings. Table 1 shows the results of this survey, sorted by total VOC emissions. Figure 1 shows this same information in graphical form, identifying water-borne and solvent-borne VOC contributions.

In developing the working groups, consideration was given to the total emissions, the size of a given category, and the similarity of formulation of coatings within a group. Table 2 shows the resulting prioritized working groups, generated using these principles.

B. Project Objectives

The overall objective of the this study was to develop improved species profiles for volatile organic compound (VOC) emissions from:

- architectural coating operations
- industrial maintenance coating operations
- associated solvent use

Pursuant to this overall goal, a number of sub-tasks were performed:

- review all information sources containing chemical composition of paint and coating materials
- specify criteria for grouping specific sources into categories
- rank source categories, based on extent of use, VOC , and other significant factors
- design, test and validate a method for accurately sampling emissions from paint and coating materials during the drying period
- collect emissions from selected paint and coating materials
- analyze the collected emissions
- compare direct emission measurements with other calculation-based methods, including literature and actual analysis of selected coating materials

II. Sample Selection

A. Classification Scheme

Since it is impossible to develop species profiles for every coating material, the formulation of "working groups" of coatings was explored. To understand historical trends in the coatings industry, three review articles were consulted:

- New Horizons in Coatings Technology, J. Coat. Technol., 63(800), September 1991
- Paints and Coatings, Chemical and Engineering News, October 18, 1993
- Organic Solvent Use, Chemical and Engineering News, June 20, 1994

Additional information on paints and coatings was obtained from the *Final Report of the Survey of Emissions From Solvent Use- Volume II: Architectural Coatings*, (September 16, 1994, ARB), and the *U.S. Paint Industry Data Base*, compiled by the National Paint and Coatings Association (September 1992).

Figure 1- Total Emissions, by Carrier

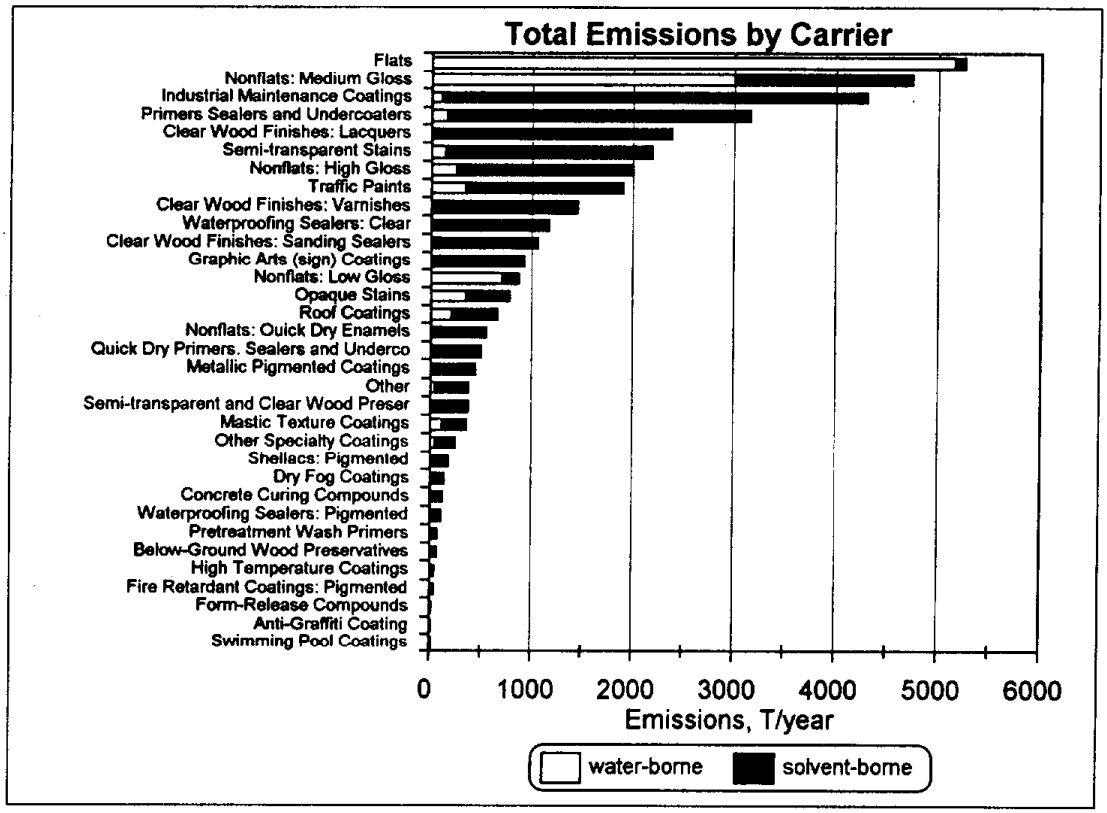


Table 1 - 1990 ARB Survey Results, Sorted by Total Emissions

category	description	Emissions (Tons/year)	% of total emissions	cum. %	WB Emissions	SB Emissions
8.0	Flats	5245	14.5	14.5	5156	89
12.0	Industrial Maintenance Coatings	4289	11.8	26.3	99	4190
17.2	Nonflats: Medium Gloss	4741	13.1	39.4	3001	1740
21.0	Primers Sealers and Undercoaters	3148	8.7	48.1	157	2991
4.1	Clear Wood Finishes: Lacquers	2378	6.6	54.7	24	2354
24.0	Semi-transparent Stains	2176	6.0	60.7	139	2037
17.1	Nonflats: High Gloss	1995	5.5	66.2	253	1742
29.0	Traffic Paints	1900	5.2	71.4	336	1564
4.3	Clear Wood Finishes: Varnishes	1437	4.0	75.4	14	1423
30.1	Waterproofing Sealers: Clear	1161	3.2	78.6	22	1139
4.2	Clear Wood Finishes: Sanding Sealers	1047	2.9	81.5	3	1044
10.0	Graphic Arts (sign) Coatings	909	2.5	84.0	1	908
17.3	Nonflats: Low Gloss	862	2.4	86.4	706	156
17.4	Nonflats: Quick Dry Enamels	548	1.5	87.9	0	548
22.0	Quick Dry Primers. Sealers and Undercoaters	495	1.4	89.3	16	479
15.0	Metallic Pigmented Coatings	440	1.2	90.5	0	440
23.0	Roof Coatings	643	1.8	92.3	206	437
18.0	Opaque Stains	767	2.1	94.4	345	422
25.0	Semi-transparent and Clear Wood Preservative	359	1.0	95.4	6	353
31.0	Other	368	1.0	96.4	44	324
14.0	Mastic Texture Coatings	339	0.9	97.3	112	227
32.0	Other Specialty Coatings	247	0.7	98.0	41	206
26.2	Shellacs: Pigmented	179	0.5	98.5	0	179
6.0	Dry Fog Coatings	130	0.4	98.8	5	125
5.0	Concrete Curing Compounds	112	0.3	99.2	18	94
30.2	Waterproofing Sealers: Pigmented	94	0.3	99.4	2	92
2.0	Below-Ground Wood Preservatives	58	0.2	99.6	0	58
20.0	Pretreatment Wash Primers	60	0.2	99.7	5	55
11.0	High Temperature Coatings	30	0.1	99.8	0	30
7.2	Fire Retardant Coatings: Pigmented	25	0.1	99.9	0	25
9.0	Form-Release Compounds	16	0.0	99.9	1	15
1.0	Anti-Graffiti Coating	14	0.0	100.0	8	6
27.0	Swimming Pool Coatings	8	0.0	100.0	0	8

The final group in Table 2 includes the solvents associated with the recommended thinning of the coating materials. Based on the data in the Final report on "The Survey of Emissions From Solvent Use, Volume II: Architectural Coatings" (September 16, 1994), thinning operations result in the release of 444 tons/year of VOC. While this is only 1 percent of the total VOC contributed by paints and coatings, ARB has expressed particular interest in this category of materials. The inclusion of this as a separate category will allow us to determine a source profile for solvents, based on the same criteria as with the other categories. The main components of this category will be mineral spirits, with a smaller contribution from VM&P naphthas. NPCA ("U.S. Paint Industry Database", SRI, September 1992, p. 145) indicates the following annual solvent usage:

mineral spirits	90 million gallons
VM&P naphtha	28 million gallons
lacquer diluents	7 million gallons

The existing species profile for Surface Coating Solvent - General (Profile 96) shows an aromatic content (xylene plus toluene) of about 8%, as shown below (reference: ARB Speciation Manual, Second Edition, August 1991):

Surface Coating Solvent Profile (96)

compound	weight fraction
acetone	0.1000
ethyl alcohol	0.0560
isomers of decane	0.2780
isomers of nonane	0.1090
isomers of octane	0.0040
isomers of undecane	0.0100
isomers of xylene	0.0400
isopropyl alcohol	0.0570
methyl alcohol	0.0560
methyl ethyl ketone	0.1000
methyl isobutyl ketone	0.0500
perchloroethylene	0.1000
toluene	0.0400
TOTAL	1.0000

The profile for composite mineral spirits (profile 802) shows a number of aromatic compounds that total 10 % of the emission profile. Rule 66 suggests that solvents with aromatic content less than 2 % should be replacing solvents of higher aromaticity. Personal communications with paint and coatings manufacturers indicate that this is the case. Mineral spirits with less than 2 % aromatic compounds appear to represent the dominant thinning currently in use in California. This suggests that profile 86 for Stoddard Cleaning Solvent (a mineral spirit) may be more typical of modern solvent usage:

Stoddard Cleaning Solvent Profile (86)

compound	weight fraction
isomers of decane	0.6930
isomers of nonane	0.2730
isomers of octane	0.0080
isomers of undecane	0.0260
toluene	0.0400
TOTAL	1.0000

Table 2 - Constitution of Working Groups

group #	working group name	material emissions (T/y)	% of all working groups	ARB categories
1	water-based flats/low gloss/medium gloss	10,371	31.3%	8.0, 17.2, 17.3
2	clear wood finishes(clear sanding sealers, watersealers, lacquers)	4,552	13.7%	4.1, 4.2, 30.1
3	solvent based industrial maintenance coatings	4,301	13.0%	12.0
4	solvent based medium gloss/high gloss	3,457	10.4%	17.1, 17.2
5	solvent based primers and sealers	2,506	7.6%	21.0
6	semitransparent stains	2,037	6.1%	24.0
7	traffic paint	1,901	5.7%	29.0
8	varnishes	1,467	4.4%	4.3
9	quick dry primers and enamels	1,246	3.8%	22.0, 17.4
10	graphic arts coatings	904	2.7%	10.0
11	thinning solvent[a]	444	1.3%	
	total of all working groups	33,186		
	TOTAL California emissions	39,063		
	% of total in all working groups[b]	85%		

[a]estimate based on manufacturer recommended thinning levels

[b]remaining total emissions are accounted for by a number of categories, each of which accounts for <1% of total VOC emissions

Table 3 - SAMPLE TYPES AND NUMBERS

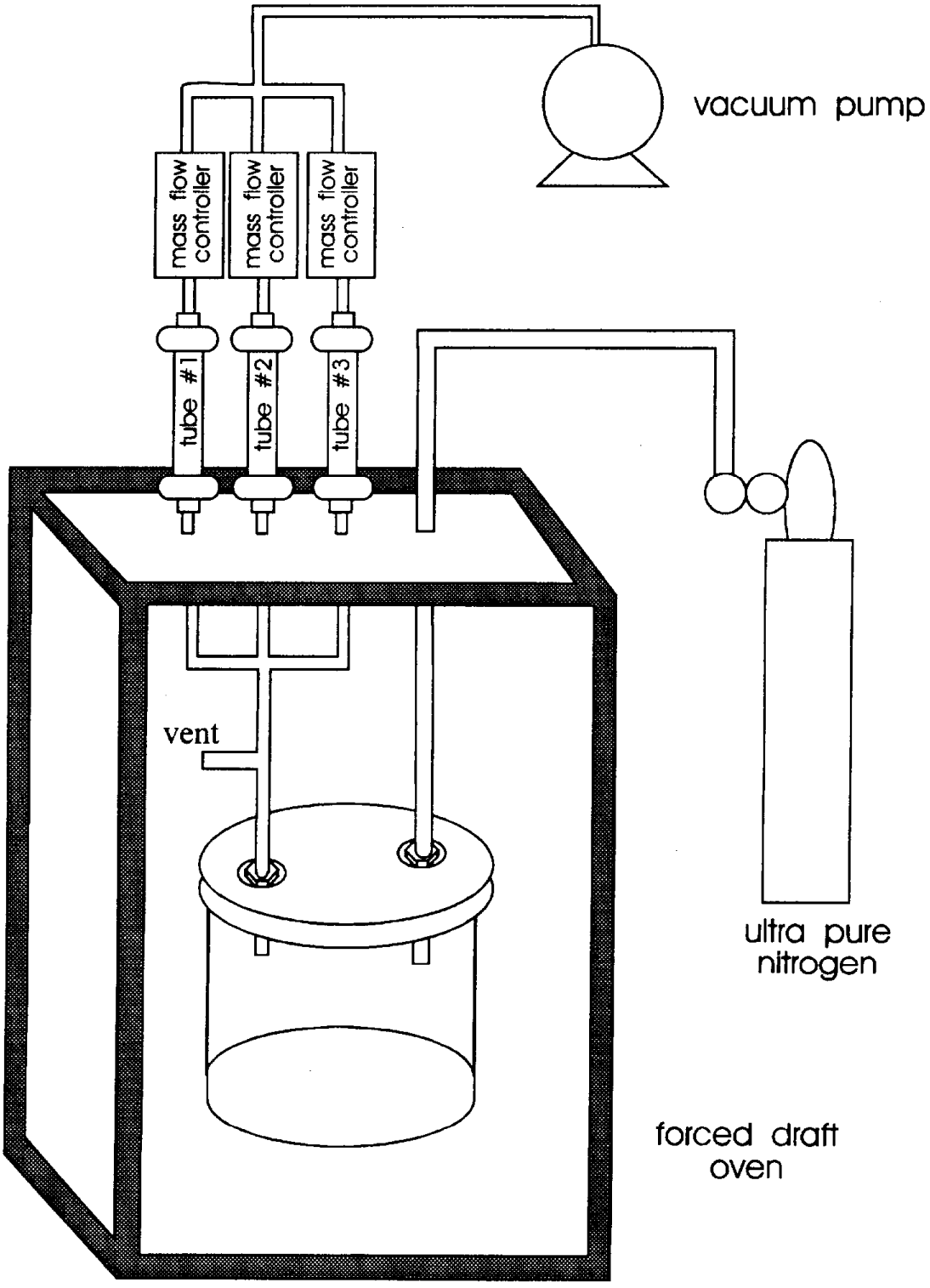
group #	working group name	% of working group	ARB categories	indicated # of samples	adjusted # of samples
1	water-based flats/low gloss/medium gloss	31.3%	8.0, 17.2, 17.3	22	35
2	clear wood finishes(clear sanding sealers, watersealers, lacquers)	13.7%	4.1, 4.2, 30.1	10	11
3	solvent based industrial maintenance coatings	13.0%	12.0	9	20
4	solvent based medium gloss/high gloss	10.4%	17.1, 17.2	7	7
5	solvent based primers and sealers	7.6%	21.0	5	5
6	semitransparent stains	6.1%	24.0	4	7
7	traffic paint	5.7%	29.0	4	7
8	varnishes	4.4%	4.3	3	4
9	quick dry primers and enamels	3.8%	22.0, 17.4	3	3
10	graphic arts coatings	2.7%	10.0	2	2
11	thinning solvent	1.3%		1	5
	TOTAL number of samples			70	106

B. Selection of Samples

To generate profiles that are representative of a given working group, coatings that correspond to the composited ARB categories were sampled. For example, the species profile for the first working group was derived from the analysis of coatings from ARB categories 8.0, 17.2 and 17.3 (water-based flats, low gloss, and medium gloss, respectively). As a starting point, the number of samples to be analyzed in each group was made proportional to the fractional contribution of the group to total VOC, as shown in Table 3. In this scheme, the number of samples taken from each sub-category would be proportional to the total VOC (tons/year) of each sub-category. This procedure resulted in a comparatively low number of samples from some groups containing diverse coating types (such as the Industrial Coatings Group, comprising at least ten distinctively different types of coatings). The adjusted number of samples analyzed in each Group is shown in Table 3. The total number of samples analyzed (106) was significantly more than the 70 originally planned. Within each group, specific coating samples were chosen, with more consideration given to those coatings which were more widely used. Attempts were also made to sample multiple manufacturers, where possible.

A combination of methods was used to obtain the coating samples for emission testing. Direct retail purchases were utilized for those samples whose availability permitted. Some of the coating materials were not directly available to the consumer. Manufacturers of these materials were generally cooperative in supplying us with samples. Material Safety Data Sheets (MSDS) were requested for all coating samples, and were received for most samples.

Figure 2 - Schematic of Chamber Sampling System



III. Sampling and Analysis Methods

A. Emission Chamber Design and Testing

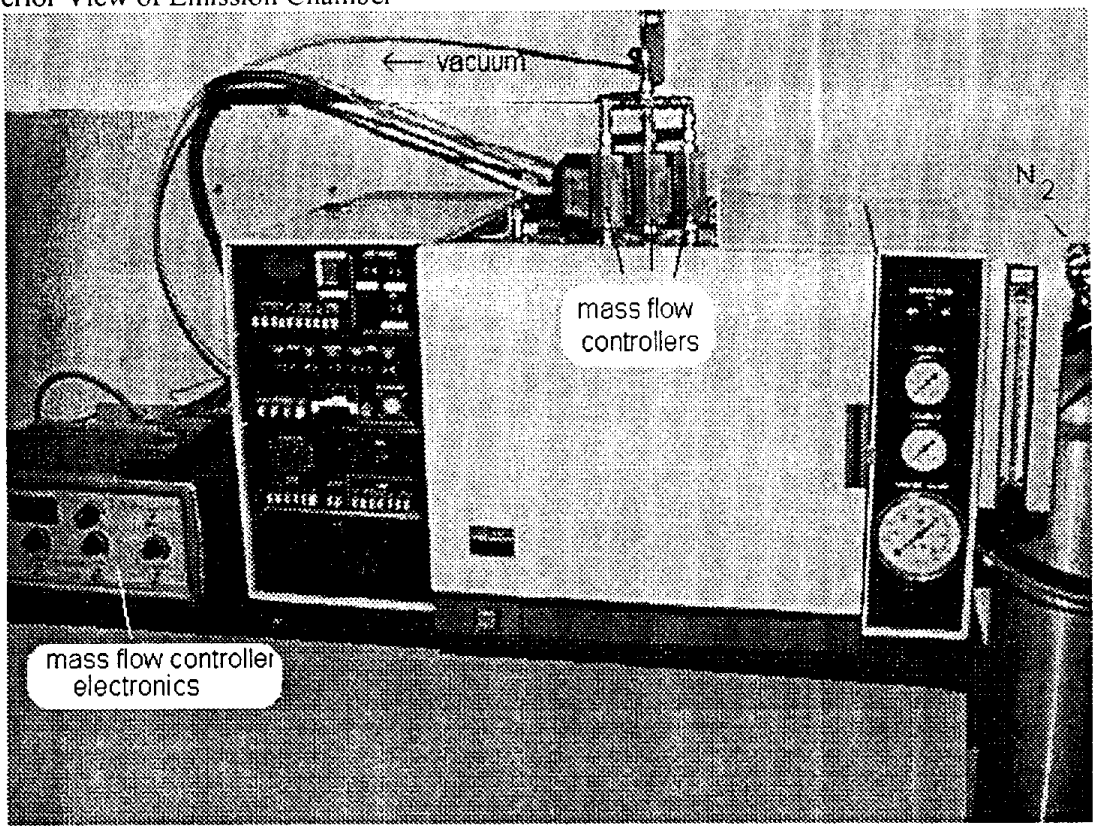
To collect the hydrocarbon emissions associated with the drying of a selected coating, a sampling chamber was constructed (a sub-task of Task 2). The chamber was fabricated from a 1 quart, friction-top metal paint can, housed in a modified forced draft oven. The lower portion of the container held the paint or coating sample, and was designed to be used only once. The can top was equipped with ¼ inch stainless steel fittings which allowed the released VOCs to be swept from the chamber by a stream of ultra-high purity nitrogen into a manifold leading to multiple sorbent tubes containing a multisorbent. A septum adapter, holding a Teflon-faced septum, was also located in the container top. Following a purge and leak check, the coating sample was injected through the septum. A number of glass beads (four or five), 10 mm in diameter, were placed in the can before sealing. These beads facilitated spreading the coating sample into a thin film. Standard Operating Procedures for use of this chamber may be found in Appendix A. A schematic diagram of the chamber sampling system is shown in Figure 2. Details of the sampling chamber are shown schematically in Figure 3. Photographs of the actual components are shown in Figure 4. The use of Teflon-seated stainless steel quick-connect fittings (Swagelok, QT series, double-ended shut off) in the oven interior allowed the sampling chamber to be easily positioned. In its final configuration, the sorbent tubes (and mass flow controllers) were the only components outside of the oven. The downstream end of the sorbent tubes were directly attached to bulkhead fittings through the roof of the oven. This design allowed for complete transfer of emissions to the sorbent tubes. The purged emissions were pulled through the sorbent tube manifold by a Teflon-faced diaphragm vacuum pump (KNF Neuberger, model N05) placed upstream of the sorbent tubes. A length of ¼ inch Teflon tubing was used to connect the vacuum pump to the upper sorbent tube manifold. Flow through each of the three sorbent tubes was regulated by a separate mass flow controller (Tylan model FC-260).

During operation, ultra pure nitrogen gas, delivered from an aluminum cylinder (Scott Marin Co.), was metered into the chamber at the rate of 1 liter per minute. The effluent from the can entered the lower stainless steel manifold. Three mass flow controllers, operated in the range of 10 to 50 mL per minute were used to direct a portion of the flow to separate sorbent tubes, where the VOCs emitted from the coating were retained. Drying times and temperatures were consistent with current practice, as outlined in ASTM Method D2369-92 (*Manual On Determination Of Volatile Organic Compounds In Paints, Inks, And Related Coating Products, ASTM Manual MNL 4, Second Edition, August 1993*), which calls for a drying temperature of 110°C for 1 hour. While there may be some question about whether the VOCs obtained from elevated drying temperatures are consistent with real-world curing cycles, the selection of a standardized temperature ensured uniformity with current regulations.

The sorbent tubes were maintained at or near room temperature, to minimize the possibility of breakthrough. A tube cooling manifold was constructed from three polyethylene "y" tubes. A lab source of compressed air was used to generate four streams of cooling air. These streams were directed at the base nuts of the sorbent tubes. The temperature of the tubes was monitored near the outlet (upper end) using a thermocouple adapter. Using this system, the temperature of the sorbent tubes was kept at or below 27 °C during the entire 1 hour run, with the oven at 110 °C. The balance of the effluent stream not led to sorbent tubes was vented through a tee located on the can top. By venting most of the effluent, overloading the sorbent was avoided. The total mass of VOCs applied to the sorbent was easily controlled by this method. The sorbent tube analyzed by GC-MS must contain a lower concentration than if it were analyzed using GC-FID, due to the requirements of the analytical instrumentation systems used. The final sampling system allowed for much versatility in terms of replicates, and sample splits.

Figure 4 - Photographs of Chamber Sampling System

Exterior View of Emission Chamber



Interior View of Emission Chamber

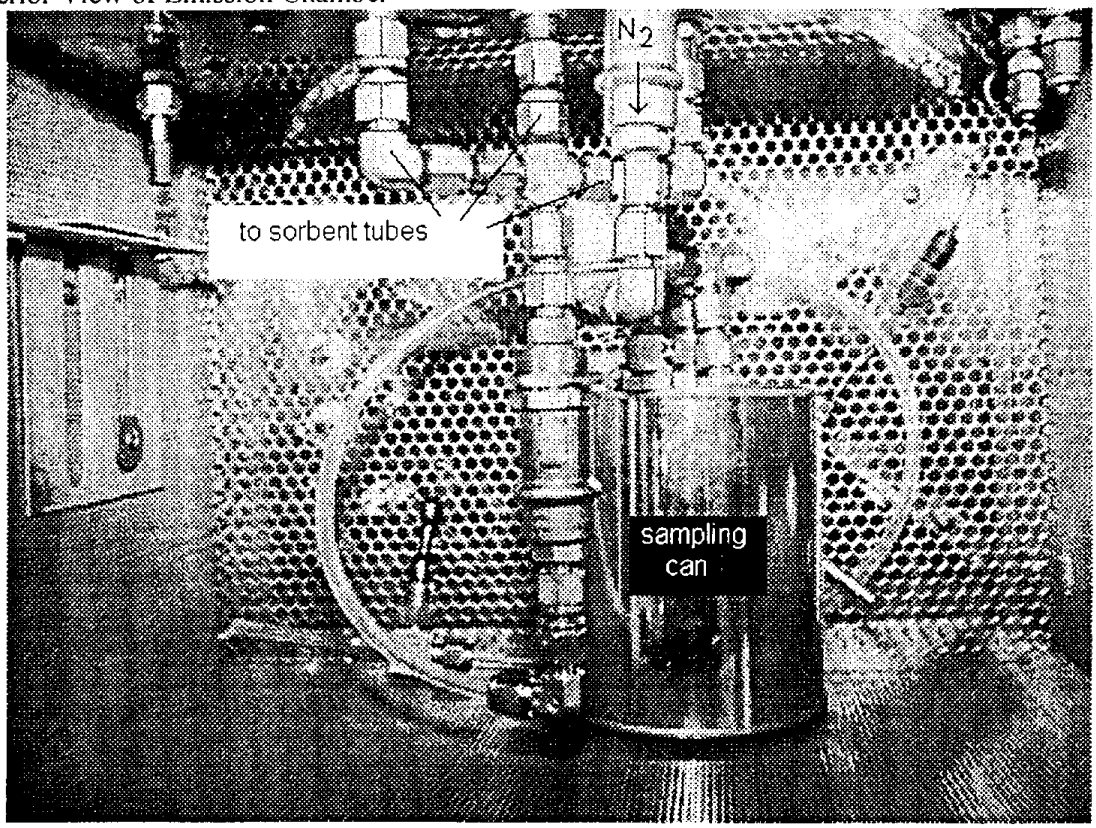
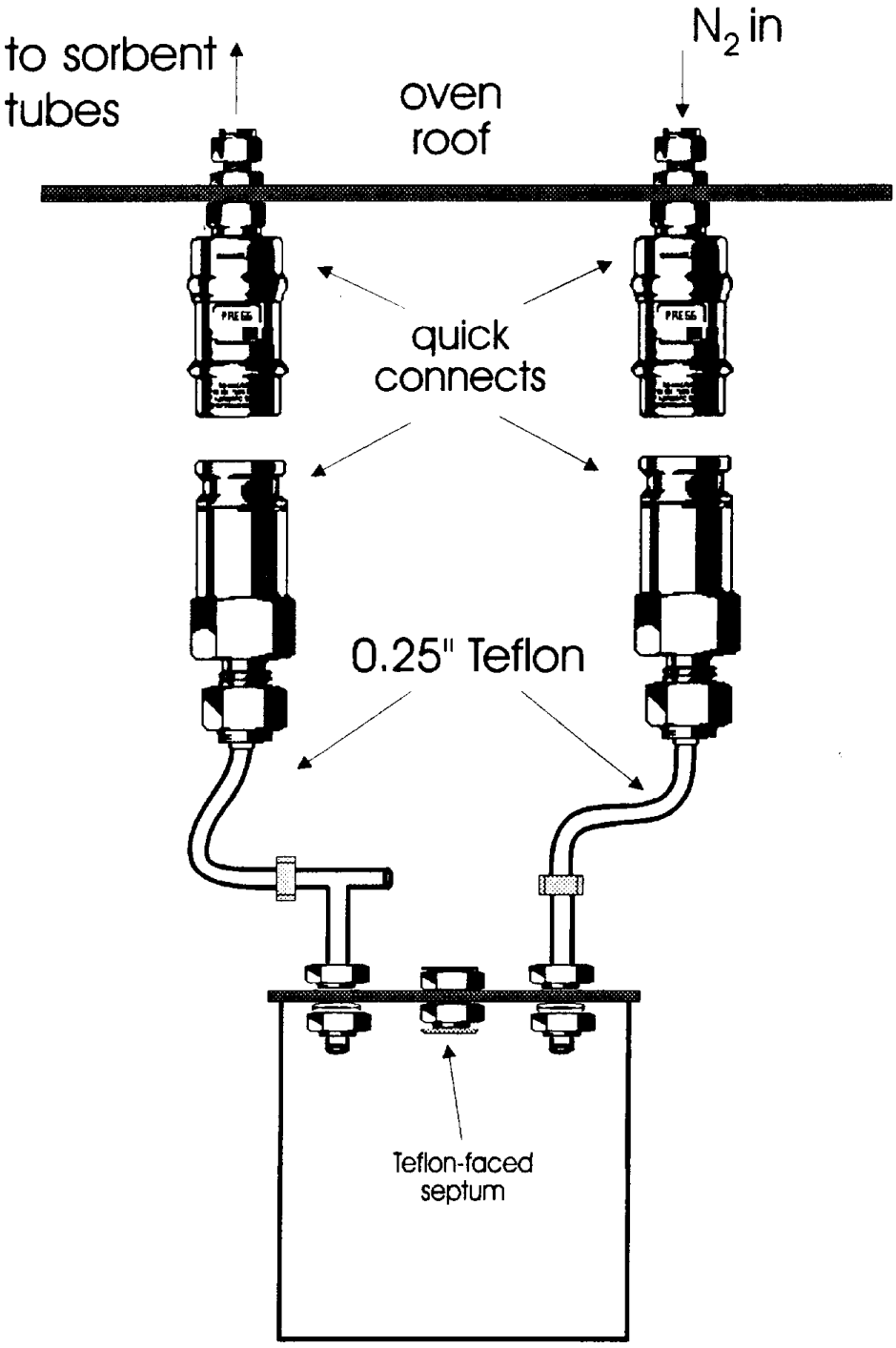


Figure 3 - Details of Chamber Sampling System



For use with a solvent desorption system, a glass sorbent tube (Supelco, ORBO Tube #100) was selected for evaluation. This tube contains two separate beds of Carbotrap (graphitized carbon black). The main portion contains 350 mg of 20/40 mesh Carbotrap, while the backup section contains 175 mg of the same sorbent. This tube was selected for comparability with the stainless steel Carbotrap 300 tube (thermal desorption unit), described previously. The stock ORBO tube has physical dimensions similar, but not identical, to the thermal desorption units investigated. The outer diameter of the glass ORBO tube is 7 mm (vs. 0.25" for the stainless steel tube). Figure 6 shows a comparison of the two tube configurations. This size difference required some modifications in the sampling system. The final configuration involved drilling out 0.25" Swagelok nuts with a 0.281" drill. Matching Teflon ferrules were similarly drilled out. This configuration provided a reliable connection to the stainless steel sampling manifold and mass flow controllers. When sampling with stainless steel sorbent tubes, we found that the three stainless steel sorbent tubes provide adequate support for the mass flow controllers. It was not clear that the glass tubes would offer sufficient support for the mass flow controllers. In the final configuration, either two empty 0.25" stainless steel tubes could be used for the outer arms of the sampling manifold, or a stainless steel support tube could be used in the middle arm, allowing for the use of two glass sorbent tubes. Eventually, the tube manufacturer was able to supply us with custom tubes, in 0.25" diameter, allowing for better integration into the steel sampling system with standard sized ferrules.

With the sampling system fully assembled, a dummy run was performed, using ultrapure nitrogen as sweep gas through a modified 1 quart paint can. The pressure in the can was monitored by a Magnehelic gauge (0-10" H_2O). At the nominal flow rate of 1000 mL/min, the pressure drop across the can was only 0.1" H_2O. Thus, the emissions from coating samples in the can were evolved at essentially atmospheric pressure.

During this run, the temperature INSIDE the can was monitored by a thermocouple suspended in the middle of the can. Just before the start of the run, the can was placed inside the oven, which was at ambient temperature, and the sweep flow of nitrogen was established. When the oven was commanded to 110°C, it required about 2 minutes to reach and stabilize at the set point. During the heating, the temperature of the can lagged behind. At t = 1.00 minute, the oven was at 86 °C, while the can interior was at 64°C. At t= 2.00 minutes, the oven had reached 100°C, while the can interior was at 94°C. At t= 5 minutes, the can interior was at 109°C. By t = 6 minutes, the can had reached 110°C. During the entire 1 hour run, the temperature inside the can was within 0.2 degrees of the oven temperature. As a result of this test, plans to pre-heat the nitrogen before leading it into the can were abandoned. The surface of the paint can appears to efficiently heat the nitrogen as it flows into the can, at least at the flow rates used for our investigation.

B. Sorbent Tube Designs

The VOCs emitted from paint and coating samples cover a wide range of boiling points and polarities. A single sorbent cannot effectively absorb and retain both low- and high boiling compounds. For this reason, a multi-sorbent was selected for this study. Pre-packed ¼ inch stainless steel sorbent tubes containing Carbotrap 300 are commercially available. (Supelco, ORBO tube #100). A schematic of this multi-sorbent tube is shown in Figure 5. The following information on the nature of the sorbents used in the tubes is provided by the tube manufacturer.

> *The Carbotrap C and Carbopack C adsorbents used in Carbotrap adsorbent tubes differ in mesh size only (20/40 mesh and 60/80 mesh respectively) and have a surface area of approximately 10m^2/gram. Researchers at Supelco have found that, relative to other adsorbents, Carbotrap C and Carbopack C have superior trapping ability for a wide variety of C12 and above (depending on molecular size and shape) organic contaminants for both air sampling and purge and trap applications.*
>
> *Carbotrap B and Carbopack B adsorbents used in Carbotrap adsorbent tubes differ in mesh size only (20/40 mesh and 60/80 mesh respectively) and have a surface area of approximately 100 m2/gram. Researchers at Supelco have also found that relative to other adsorbents, Carbotrap and Carbopack B have superior trapping ability for a wide variety of C5 and above (depending on molecular size and shape) organic contaminants for both air sampling and purge and trap applications. Studies of thermal desorption are an ongoing effort at Supelco.*
>
> *Carbosieve S-III spherical carbon molecular sieve has a large surface area (about 800 m^2/gram) and 15 to 40 angstrom pores. This structure makes Carbosieve S-III adsorbent very useful for trapping small molecules such as vinyl chloride. The pure carbon framework allows thermal desorption of small analytes without loss.*

Compounds with carbon numbers ranging from C2 to over C12 are effectively sorbed by the combination of three sorbents used in the Carbotrap 300 tubes. Both ends of each tube were Swaged into ¼ inch stainless steel bulkhead fittings. An identification number was engraved onto each tube. These tubes were designed for thermal desorption into a chromatographic inlet system. Early on in our investigation, we began to explore the use of solvent desorption, in parallel with thermal desorption techniques.

Figure 6 - Comparison of Two Sorbent Tube Types

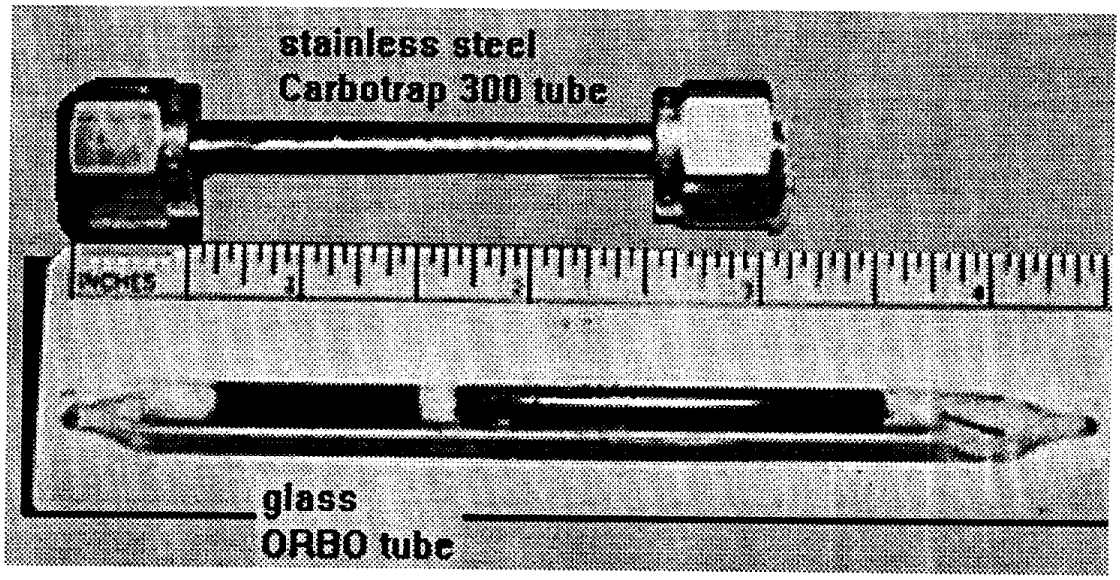
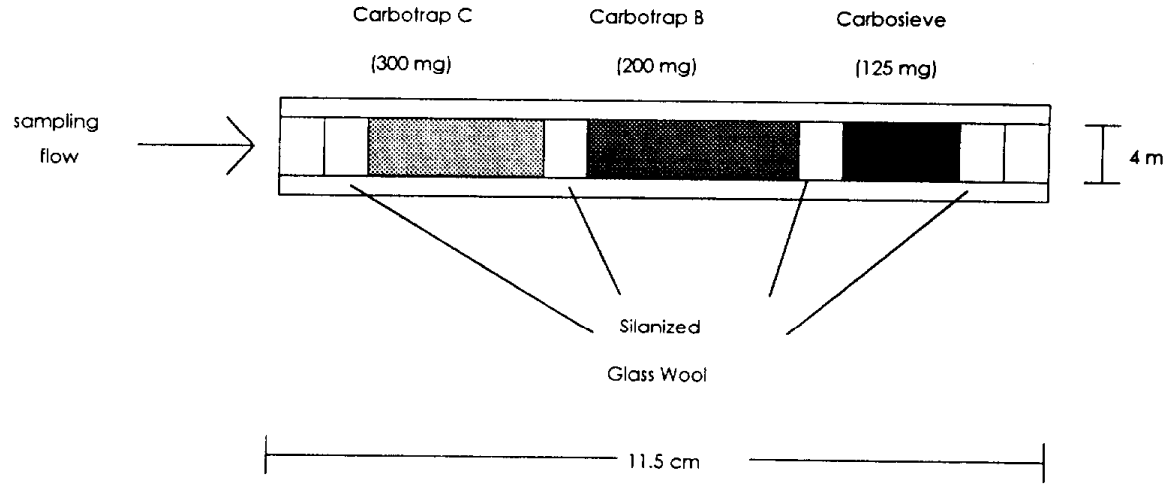


Figure 5 - Carbotrap 300 Sorbent Tube

Adsorbate	Desorption Efficiency ± %RSD
Benzene	100 ±5.5
Bromoform	100 ±2 1
Carbon tetrachloride	99 ±3.6
Chlorobenzene	100 ± 0.7
Chloroform	94 ±5.2
3-Chloropropene	100 ±3.2
Cumene	99 ±3.6
1 ,2-Dichloroethane	102 ±4.1
1, 1 -Dichloroethane	101 ±0.6
Dichloromethane	98 ±10
Ethylbenzene	100 ±3.0
n-Heptane	99±4.2
1 -Heptene	99 ±4.7
Tetrachloroethylene	99 ±2.9
Toluene	99 ±4.2
1 1,1,1-Trichloroethane	100 ±3.0
Trichloroethylene	101 ±2.6
Vinyl chloride	101±2.5
o-Xylene	99 ±3.6
m-Xylene	100 ±3.8
p-Xylene	99±3.6

Reference: Supelco GC Bulletin 849B



3. Recovery of Target Analytes from Stainless Steel Sorbent Tubes

To ensure that the sampling chamber does not act as a sink for VOC emissions, the recovery of compounds expected in coating samples was examined. We added a known amount of an aqueous standard containing ethylene glycol, propylene glycol, butyl carbitol, and butyl cellosolve (approximately 1% in each component, dissolved in Type I water), and proceeded to sample the chamber emissions, in accordance with sampling and analysis SOPs. Since these components were seen to yield poor response on a mass spectrometric detector, they were run by thermal desorption in the sub-contractor's laboratory, using a GC-FID system. This standard four component mixture produced four chromatographic peaks, but with poor peak shapes. Apparently, these highly polar compounds were being retained and broadened by the chromatograph's sample inlet system. For the initial testing phase, we selected what we believed to be worst-case solvents, that is, those for which difficulties had been reported in previous studies. Indeed, these solvents proved troublesome in our initial testing. We proceeded to explore an alternative to the thermal desorption method for analyzing emissions containing solvents found in typical water-based coatings.

D. Solvent Desorption Procedures

Dr. Max Wills investigated and refined a procedure for determining the VOC content of paints and coatings by analysis of the solvent extracted glass sorbent tubes. The procedure, and its initial results, are reported in the sections below.

1. Work-up procedure

Following sampling, the upper retaining cotton plug and section B of the ORBO tube consisting of 175 mg of Carbotrap were placed in a 15 x 1.5 cm screw-capped test tube. The lower section (Section A, 350 mg Carbotrap), including both cotton retaining plugs, was pushed into a separate test tube using a wooden applicator stick. The empty ORBO tube was also placed into the test tube. The test tubes were sealed and methanol (MeOH) containing 0.1058 mg/mL of 2-ethylhexanol as internal standard (IS) was added. The contents were manually mixed, then sonicated for 15 minutes and centrifuged. This extract contained all of the solvents in the original coating sample, but none of the pigment or polymer, which were left behind, in the chamber can bottom.

A 2 μL aliquot of the centrifugate was injected into a Hewlett Packard gas chromatograph (model 5890), equipped with a flame ionization detector. The column used was a 15m x 0.53 mm SE-30 (Econocap, Alltech) capillary column. The injection port was maintained at 240°C, the FID detector at 280°C. The oven temperature was programmed from 50°C for 2 minutes, to 230°C, at 30°C per minute, with a hold at 230°C for 2 minutes. The split injection technique was used initially, but splitless injection eventually proved to be superior.

C. Chamber Validation Studies

Before using the chamber to obtain species profiles, a number of experiments were performed to validate its design and suitability to the task at hand. The various types of experiments conducted are described in detail below.

1. Blank Determinations

The VOC background in the entire sampling system must be low enough to allow VOCs from small amounts of coatings to be readily detected, with minimal interference from ambient sources. Sources that contribute to the "background" VOC level include the nitrogen purge gas, the sampling chamber, and sorbent tubes.

For all chamber tests, the source of the purge gas was high purity nitrogen gas, obtained by evaporation of liquid nitrogen, and stored in aluminum cylinders. This gas was purchased from Scott-Marin, Inc. Since this grade of nitrogen is used to prepare certified reference mixtures of gases, it should not contribute measurable amounts of VOC to the sampled emissions. To assess the total background, blank runs were performed, using the same SOP used for sampling, but without any added coating sample. The sampling chamber was assembled, and purged with high purity nitrogen , with the oven at ambient temperature. The oven was heated to 110^{o}C, and the emissions were collected on cleaned, conditioned sorbent tubes for a period of one hour. For the blank runs, two of the mass flow controllers (MFC) were operated at a flow of 10 mL per minute, and the third MFC was operated at a flow rate of 50 mL per minute. The larger flow rate in the third MFC allowed for higher sensitivity for the blank determination. Following a 1 hour sampling time, the ends of the sorbent tubes were sealed with brass caps, and the sorbent tubes were stored in a glass jar, pending transportation to the analytical laboratory. Subsequent analysis of these tubes by thermal desorption into a gas chromatograph equipped with a flame ionization detector (GC-FID) revealed no measurable peaks, indicating the validity of the cleaning/conditioning protocols. The desorption procedure was that detailed in EPA Method TO2 (Compendium of Methods for the Analysis of Air Toxics). Blanks were obtained for several unused sorbent tubes. The chromatograms from these sorbent tubes were essentially indistinguishable from the chamber blank runs. By this series of tests, the cleaning process used for the sampling chamber was shown to be sufficient to produce a clean background.

2. Variability of the Sampling Manifold

To assess the uniformity of the splits obtained with the sampling manifold, a known amount of an aqueous butyl carbitol standard was added into our normal 1 quart emission can, and the purged material was collected in three stainless steel Carbotrap 300 sorbent tubes, using our normal sampling system. These samples were successfully analyzed by thermal desorption, and provided a good test of tube-to-tube variability. Two sorbent tubes in different mass flow controller arms, operated at the same flow rate (10 mL/min) produced peak areas for butyl carbitol that were within 2% of each other.

The calculation method for GC runs may be expressed as:

$$\text{Analyte \%} = [(AA \times RF)(VS \times DF)/(AIS \times WS)] \times 100$$

where
- AA = area response of analyte.
- RF = response factor for analyte in mg analyte per area unit relative to the unit area response for an internal standard concentration of 1.0577 mg/mL of 2-ethylhexanol.
- VS = volume of MeOH/IS
- DF = dilution factor for MeOH/IS
- AIS = area response of internal standard
- WS = weight of sample in mg

Chamber test W-03 was conducted using a well-characterized latex paint, RS-054. The chamber effluent was passed through the ORBO tube at a flow of 35.0 mL/min for 1 hour, with the oven at 110°C. Based on the initial sample weight of 0.3200g, the amount of sample going to the ORBO tube was 3.5% (35 mL/min out of 1000 mL/min) of 0.3200g , or 11.20 mg.

Both sorbent sections were initially extracted with 5 mL MeOH/IS (concentration of IS = 0.10577 mg/mL) and gas chromatographed as described above. After chromatographing this solution, an additional 5 mL portion of MeOH/IS was added to the test tube containing the sorbent and previous extractant. The contents were again sonicated and centrifuged and then chromatographed again. The results for these analyses are shown in Table 5.

From the data in Table 5, it appears that an extraction volume of 10 mL of MeOH/IS was more efficient than a 5 mL volume, indicating that analyte may be retained by the Carbotrap when smaller volumes of solvent are used for extraction. This sample contained a wider dynamic range of solvent concentrations than the previous sample. Consequently, the size of the chromatographic peaks for the minor components (EG and Texanol, TX) was quite small, producing some uncertainly in the integration process. Based on the results for this sample, it would have been better if a larger sample size were taken. Since breakthrough was not observed in the upper sorbent section of this sample tube, a larger sample size could have been easily accommodated. For subsequent runs, sample mass was increased for those samples having components lower in concentration than 1%. The bottom of the paint can sampling chamber was examined after the sampling run. A thin film of dried paint was observed on the can bottom. Scraping this deposit with a steel spatula showed that it was fully dried, with no apparent trapped liquid paint.

The resulting emission profile, calculated from the average of the 10 mL extraction runs, is shown in the lower half of Table 5.

For the emission chamber results for sample W-02 (see Table 4), excellent results were obtained for the aqueous standards, indicating the validity of the sampling and analytical procedures. For the paint samples, however, results were systematically low for some of the less volatile components, such as butyl carbitol and Texanol. We explored the nature of these apparent losses in the following sections. The agreement between experimental and actual weight fractions for the major component is excellent. The poorer agreement for the minor components is attributable (at least in part) to the small peaks obtained during the chromatography. This was a consequence of the initial sample mass selected.

Some difficulty was encountered in dealing with the small areas produced by chromatographic peaks of minor (<1%) components. A new injection method, utilizing a splitless technique was seen to significantly improve the size of these minor peaks. Results for the initial set of chamber tests are given in Table 6. Results from the direct analyses (described in Part E) are shown in Table 7. Some comparative results are illustrated in Table 8.

2. Blank Determinations

An unused ORBO tube was randomly selected from a lot of ten to serve as a blank. Both ends of the tube were scored, using a rotary emery disk, and the tube ends broken off. The tubes ends were then sealed with end caps, as with other samples, and the capped tube was placed into a screw-capped test tube. The upper section (Section B) of sorbent in this tube was discarded; section A was worked-up in the same manner as other samples and diluted with 10 mL of MeOH/IS(0.10577 mg/mL 2-EH). Chromatography at fairly high FID sensitivity showed no peaks corresponding to VOC species expected to be found in coating samples. Several small peaks attributed to impurities in the MeOH/IS solution were observed in this as well as for runs with other coating samples. Two small peaks observed at long retention times were determined to be system peaks (artifacts) which were impurities in the injector which become flushed onto the column whenever an injection was made. Since these peaks were observed long after any analyte peaks were observed, they did not interfere with the subsequent interpretation of the chromatograms. From this set of experiments, we concluded that the initial blank level of the ORBO tubes as received from the manufacturer was acceptable, and that normal handling of the sorbent tubes (consistent with the SOPs used) did not produce any detectable contamination of the tube.

3. Validation Tests for Solvent Desorption Method

To assess the efficacy of the solvent desorption procedure, a chamber test (sample W-02) was conducted, using an aqueous standard containing ethylene glycol, propylene glycol, butyl carbitol, and buytl cellosolve (about 1% each in Type I water). The chamber effluent was passed through the ORBO tube at a flow of 35.0 mL/min for 1 hour, with the oven at 110^{o}C. Based on the initial sample weight of 0.4637g, the amount of sample going to the ORBO tube was 3.5% (35 mL/min out of 1000 mL/min) of 0.4637g , or 16.23 mg.

Following sampling, each sorbent section was extracted separately with 10 mL MeOH/IS (concentration of IS = 0.10577 mg/mL) and gas chromatographed as described above. The only peaks observed were those belonging to the analytes known to be present in the sample. This indicated the lack of contamination in the sampling system and purge gas supply. Table 4 shows the results of the analysis for the lower (main) sorbent section for this sample.

These results indicate good agreement between the calculated and actual composition of the sample. Based on the agreement between the found and actual compositions, there was no evidence of loss of material on the walls of the sampling chamber, nor the associated sampling lines. Recovery of all analytes was essentially quantitative. These quantitative comparisons were obtained by calculating the dynamic volumetric dilution of the chamber purge gas.

When treated identically, the upper sorbent section showed no chromatographic peaks, indicating the lack of sorbent breakthrough at the experimental conditions. Under these conditions, only about 0.652 mg of analytes was sorbed by 350 mg of Carbotrap.

Based on these results, a species profile may be generated for this sample. Such a profile is shown in the lower half of Table 4. The agreement between found and actual emission profiles was good.

Table 5 - Results for Chamber Sample W-03 (Latex Paint RS-054)

Analyte	Coating Composition Found (%)				Actual (%)
	Extracted with 5 mL MeOH/IS		Extracted with 10 mL MeOH/IS		
	GC Run 1	GC Run 2	GC Run 1	GC Run 2	
EG	0.63	0.51	0.57	0.57	*0.59*
BuCA	10.40	10.50	11.04	11.06	*11.08*
TX	0.40	0.34	0.44	0.46	*0.59*

Analyte	Emission Wt. fraction	
	(10 mL average)	Actual
EG	0.0474	*0.0481*
BuCA	0.9151	*0.9038*
TX	0.0375	*0.0481*
TOTAL	1.0000	*1.0000*

Table 4 - Results for Chamber Sample W-02 - Splitless Injection

Analyte	Coating Composition Found (%)			Actual (%)
	GC Run 1	GC Run 2	Average	
EG	0.92	0.99	0.96	*1.00*
PG	1.05	1.09	1.07	*1.02*
BuCE	1.16	1.16	1.16	*1.02*
BuCA	1.19	1.19	1.19	*1.00*

Analyte	Emission Weight Fraction	
	Calculated	Actual
EG	0.2183	*0.2475*
PG	0.2720	*0.2525*
BuCE	0.2446	*0.2505*
BuCA	0.2651	*0.2475*
TOTAL	1.0000	*1.0000*

Splitless injection technique

Table 7 - Emission Profiles, Direct Method

component	RS-052		RS-053		RS-054	
	experi-mental	***true***	**experi-mental**	***true***	**experi-mental**	***true***
ethylene glycol	0.5512	*0.5000*	0.0459	*0.0478*	0.0438	*0.0481*
propylene glycol	0.0000	*0.0000*	0.0000	*0.0000*	0.0000	*0.0000*
butyl carbitol	0.0000	*0.0000*	0.9110	*0.9043*	0.9100	*0.9038*
butyl cellosolve	0.0000	*0.0000*	0.0000	*0.0000*	0.0000	*0.0000*
Texanol	0.4488	*0.5000*	0.0431	*0.0478*	0.0462	*0.0481*
TOTAL	**1.0000**	***1.0000***	**1.0000**	***1.0000***	**1.0000**	***1.0000***

Table 6 - Summary of Results for Chamber Emission Profiles

	W02 (0.4637 grams of std.)		W03 (0.3200 grams of RS-054)		W04 (1.3653 grams of RS-052)		W05 (3.1287 grams of RS-054)	
component	experi-mental	*true*	experi-mental	*true*	experi-mental	*true*	experi-mental	*true*
ethylene glycol	0.2183	*0.2475*	0.0474	*0.0481*	0.5577	*0.5000*	0.0433	*0.0481*
propylene glycol	0.2720	*0.2525*	0.0000	*0.0000*	0.0000	*0.0000*	0.0000	*0.0000*
butyl carbitol	0.2651	*0.2475*	0.9151	*0.9038*	0.0000	*0.0000*	0.9215	*0.9038*
butyl cellosolve	0.2446	*0.2505*	0.0000	*0.0000*	0.0000	*0.0000*	0.0000	*0.0000*
Texanol	0.0000	*0.0000*	0.0375	*0.0481*	0.4423	*0.5000*	0.0335	*0.0481*
TOTAL	1.0000	*1.0000*	1.0000	*1.0000*	1.0000	*1.0000*	1.0000	*1.0000*

4. Effect of Sample Size

A series of tests was performed, using latex paint RS-054, to investigate the effect of sample mass on the resulting emission profiles. Our original intent on performing this study was to determine a safe sample mass, that did not produce sorbent breakthrough. For run W03, 0.3200 grams of paint was used. No solvents were detected in the upper portion of the sorbent tube. Test run W05 was performed, using 3.1287 grams of coating sample RS-054. Once again, all of the sample components were retained in the lower portion of the ORBO sorbent tube; nothing was present in the upper portion of the sorbent. The selected sorbent appears to have a high affinity for these compounds. Since they have such high boiling points, breakthrough is not a problem, even with very large sample sizes. Examination of the results (Table 6) from these two runs showed an obvious discrepancy in the emission profile for Texanol, and a minor discrepancy for butyl carbitol. The effect was somewhat more pronounced in the run with larger sample size. The presence of these solvents in the dried paint film was confirmed by analysis of the film. This procedure is described in a later section. This study led to the conclusion that the sample mass must be kept comparatively low (in the range of 0.50 grams), in order to prevent the entrapment of high boiling solvents in a thick paint film.

E. Direct Analysis of Water-Based Coating Materials

1. Sample Preparation, Non-Methanol - Containing Paints

A direct method of analyzing the bulk coating material was developed. The basis for the method involved the dilution of the coating sample with methanol and an internal standard, followed by centrifugation and gas chromatography of the centrifugate. In this method, a 10.0 mL of aliquot of methanol containing 1.0577 mg/mL of 2-ethylhexanol as internal standard was pipetted into a 20 mL screw-cap test tube with a Teflon-lined cap. Approximately 0.15 to 0.20 g paint was weighed to the nearest 0.0001 gram, by difference, directly into the methanol solution by means of a disposable Burrell pipet. The screw-cap was attached to the tube, and shaken by hand for about one minute. The tube was then placed in a sonicator for 15 minutes and then centrifuged for 10 minutes. This procedure gave an almost clear supernatant liquid for most coating samples, with the majority of the pigment at the bottom of the test tube.

Method Validation

In order to assess the accuracy of our proposed method for determining VOC content of paints and coatings by direct analysis, two well-characterized water-based paints (referred to earlier) were analyzed by direct injection onto a gas chromatograph. These paints were formulated to contain the known VOCs ethylene glycol, butyl carbitol and Texanol. The theoretical VOC values for these paints and the results found by three laboratories (Cal Poly, SCAQMD, and US Testing Company) using EPA 24 are shown in Table 9.

The GC was used in the split mode, with an injection port temperature of 240°C. The flame ionization detector was maintained at 260°C. The oven was programmed from an initial temperature of 50°C for 2 minutes, followed by a 20°C per minute ramp to 240°C. The final temperature was held for 2 minutes. The injection volume was from 2-3 μL. The column head pressure was adjusted such that ethylene glycol had a retention time of approximately 2.5 minutes. A representative chromatogram is shown in Figure 7.

As shown in Table 10, the method shows an excellent agreement with formulated values for the solvents in the tested coating materials. In addition, variability of replicate analyses seems much better than the lab-to-lab variations shown in the round-robin study, using "conventional", indirect methods for VOC determination. Based on these results, we believe that the method produces accurate species profiles. The data in Table 11 show that recovery of ethylene glycol and Texanol are reproducibly high (in the 95-96% range). Under the conditions used for the direct analysis, these solvents apparently do not become associated with the polymer phase of the coating to any great extent.

Table 8 - Comparison of Direct and Chamber Emission Profiles

	RS-052			RS-054		
component	**direct**	**chamber**	***true***	**direct**	**chamber**	***true***
ethylene glycol	0.5512	0.5577	*0.5000*	0.0438	0.0474	*0.0481*
propylene glycol	0.0000	0.0000	*0.0000*	0.0000	0.0000	*0.0000*
butyl carbitol	0.0000	0.0000	*0.0000*	0.9100	0.9151	*0.9038*
butyl cellosolve	0.0000	0.0000	*0.0000*	0.0000	0.0000	*0.0000*
Texanol	0.4488	0.4423	*0.5000*	0.0462	0.0375	*0.0481*
TOTAL	**1.0000**	**1.0000**	***1.0000***	**1.0000**	**1.0000**	***1.0000***

Calibration:

Standards containing 1.0577 mg/mL of 2-ethylhexanol (2EH) and varying amounts of ethylene glycol (EG), Texanol (TX), and butyl carbitol (BC) were prepared to establish response ratios. For each chromatogram the area of each peak was divided by the area of the 2EH peak and expressed as mg of analyte required to give the same area response as 2EH. The response was linear over the concentration range tested.

Two samples of RS-052 were prepared as described above. Weight of sample #1 = 0.1777g; #2 = 0.0859g.

One sample of latex coating RS 053 was prepared as described above. Sample weight = 0.1775 g.

The results of these analyses are shown in Table 10.

To investigate the possible recovery of solvents from the paint, a 99.75 g sample of RS 053 was weighed into a one-pint paint can, and spiked with 1.06 g of ethylene glycol and 1.04 g of Texanol and re analyzed as above. This mixture was agitated on a paint shaker for 15 minutes, to ensure homogeneity. A portion of this sample was analyzed by the direct method outlined above. The results are summarized in Table 11. The theoretical VOC concentration was recalculated using the average results from the GC analysis of unspiked RS 053.

2. Sample Preparation, Methanol - Containing Paints

Many water based traffic paints were known to contain methanol as a fast evaporating solvent. Since our direct method for analyzing water based paints by gas chromatography used methanol as the extraction solvent, it was necessary to develop a complementary method for quantifying the low boiling solvents in traffic paints. These were determined by gas chromatography of dimethylformamide (DMF) extracts of paint with 1-propanol (PA) as internal standard. PA was chosen because it has a retention time approximately in the middle of the low boiling solvents which were examined and because it is not normally used in paint formulations. Propanol was not detected in any of the traffic samples analyzed. DMF was selected as the solvent for this application, based on its good solvency for polymeric and monomeric coating materials, and its boiling point of 153°C, which resulted in its elution from the GC column well after the low-boiling solvents.

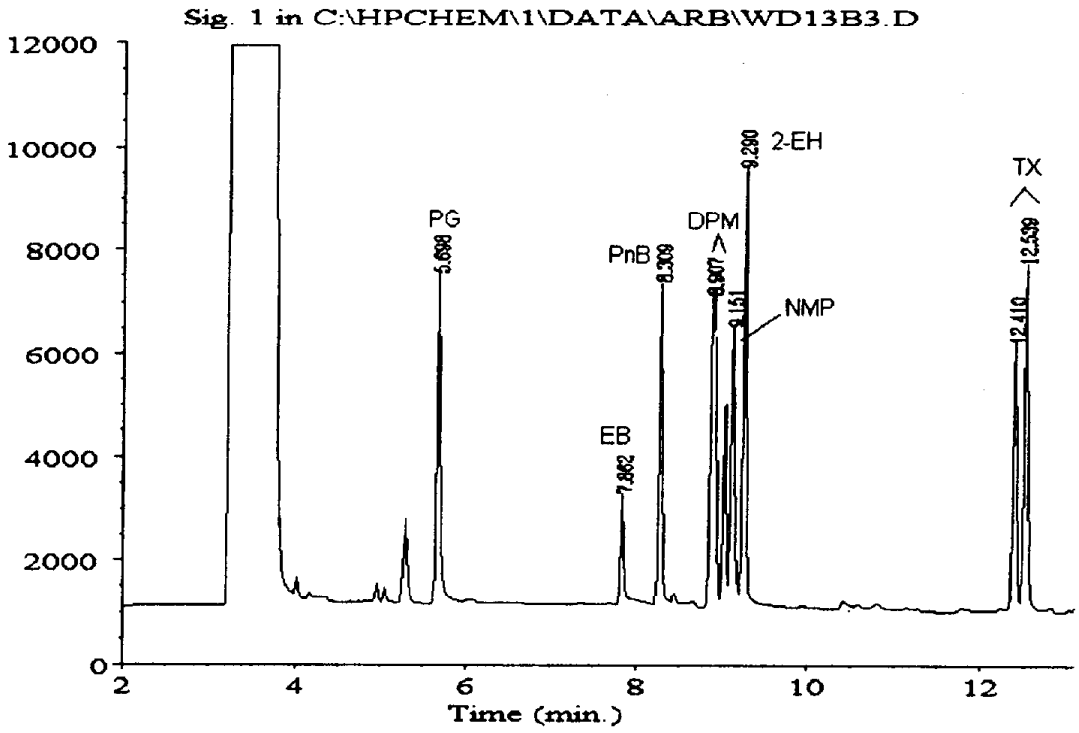
Procedure For Traffic Paints

For this method, about 500 mg of a coating sample was weighed by difference directly into 10 mL of DMF containing 1.0562 mg/mL of PA in a 20 mL screw-capped test tube. The contents were manually mixed, sonicated for 10 to 15 minutes and then centrifuged. For these analyses, a 30m x 0.32 mm SPB-1 capillary column was used. The injection port was maintained at 250 °C; detector, and the FID at 260 °C. The oven was held at 40°C for 2 minutes, then ramped to 250°C at 20°C per minute, then held at the final temperature for 10 minutes. For these analyses, split injections of 2 to 3 microliters of extract were used.

Table 9 - Theoretical and Experimental VOCs in Standard Latex Paints

Theory (Formulation Values)					Found by EPA 24		
Sample	Ethylene Glycol	Texanol	Butyl Carbitol	Total VOC, Theory	Total VOC, Lab A	Total VOC, Lab B	Total VOC, Lab C
RS052	1.06%	1.06%	0.00%	2.12%	1.31%	2.35%	1.57%
RS053	0.33%	0.33%	6.24%	6.92%	6.98%	6.41%	6.55%
RS054	0.59%	0.59%	11.08%	12.26%	12.77%	11.60%	12.52%

Figure 7 - Chromatogram of Water-Based Coating, Direct Method



Response Factors

Response factors relative to PA were established for methanol, ethanol, isopropyl alcohol, 2-butanol, methoxypropanol, and triethyl amine. Solutions of these compounds at a concentration of approximately 1 mg/mL were analyzed using the split injection technique. Response factors were calculated using the relationship:

RF = (S)(AN)/(N)(AS) where S = concentration of standard in mg/mL
AN = area response of analyte
N = concentration of analyte in mg/mL
AS = area response of standard

RF values obtained were as follows:

component	Response Factor
MeOH	0.5416
EtOH	0.7515
IPA	0.8539
2BuOH	0.9684
PM	0.6533
TEA	1.1928

Validation

A sample of traffic paint of known composition was analyzed using the DMF extraction method. Results for this paint were as follows:

Analyte	Found, %	Reported, %
Methanol	2.13	2.13
Texanol	1.78	1.63

3. Paint film Analysis

To explore the possibility that some high boiling solvents might remain associated with the polymer phase under certain conditions, we examined the dried film remaining in the sampling can after chamber run W-05. The bottom of the paint can was removed, and a portion of the dried paint film was analyzed for possible residual solvent. About 200 mg of the dried paint film was removed from the bottom of the sampling can. The weighed coating was sonicated for 30 minutes with 5 mL of acetone. Next, 5 mL of a methanolic solution of 2-ethylhexanol was added, and the mixture was sonicated for another 30 minutes. This sample was centrifuged, and the centrifugate was analyzed by GC, using our direct method. Analysis revealed that the paint film contained measurable amounts of butyl carbitol and Texanol, but no ethylene glycol. Using the known solids content of this sample (37.3%), the total amount of solvent trapped in the entire paint film could be calculated. Results are shown in Table 12. It is evident that these solvents remained in the paint film, even after the aggressive drying conditions (1 hour at 110°C) used in our chamber studies. To our knowledge, this is the first reported study of solvents remaining in the paint film after a drying period consistent with ASTM 2369. It should be noted that a large sample size (>3 grams) was used in the test. Normally, the chamber runs were conducted using coatings in the 0.50 gram range. Clearly, the thicker the paint film, the more probable it is that high boiling solvents will become associated with the film phase.

Table 11 - Recovery Study of Ethylene Glycol and Texanol from RS 053

GC Run	% EG	% TX	% BC	% Total VOC, Found
1	1.28	1.32	6.08	8.68
2	1.23	1.21	5.99	8.43
3	1.31	1.37	6.65	9.33
4	1.23	1.28	6.35	8.86
5	1.18	1.19	5.96	8.33
Average	1.25	1.27	6.21	8.73
Actual	*1.29*	*1.32*	*6.15*	*8.76*

% Recovery, EG = [(1.25 - 0.25)/(1.29 - 0.25)] x 100 = 96%

% Recovery, TX = [(1.27 - 0.31)/(1.32 - 0.31)] x 100 = 95%

Table 10 - Results of Direct Analysis of Two Latex Coatings by GC-FID

RS 052	% EG	% TX	% Total VOC, Found
Sample #1	1.03	1.03	2.06
	1.01	1.01	2.02
Sample #2	0.96	0.96	1.92
	1.05	1.05	2.10
Actual	*1.06*	*1.06*	*2.12*
Found by EPA 24			1.31, 2.35, 1.57

RS 053	% EG	% TX	% BC	% Total VOC, Found
GC Run 1	0.25	0.31	6.38	6.94
GC Run 2	0.25	0.31	6.17	6.73
Actual	*0.33*	*0.33*	*6.24*	*6.92*
Found by EPA 24				6.98, 6.41, 6.55

Table 12 - Analysis of Solvent in Paint Film

	% composition				emission factor	
	Found in sorbent	Found in film	Total Found	True	Total Found	True
ethylene glycol	0.49	0.00	0.49	0.59	0.0420	0.0481
butyl carbitol	10.33	0.36	10.69	11.08	0.9152	0.9038
Texanol	0.38	0.12	0.50	0.59	0.0428	0.0481

4. High Boiling Paint Solvent Evaporation Rate Study

As reported earlier, some high boiling solvents have been seen to remain in the paint film after one hour of drying at 110°C. We undertook a study to evaluate the significance of this phenomenon for three solvents: Texanol, dibutyl phthalate and dioctyl phthalate. Texanol (2,2,4-trimethyl-1,3-pentanediol monoisobutyrate) is one of the most common coalescing solvents for latex paints. This solvent has a reported atmospheric pressure boiling point of 244-247°C. The amount of this solvent may be determined by direct gas chromatography of paints extracted with an appropriate solvent. The total VOC content of paints as determined by EPA Method 24 involves the determination of total volatile content by heating a 0.3 to 0.5g sample of paint for one hour at 110°C (ASTM Method 2369). Evidence from studies in which the volatile portion of paint is collected in charcoal sorbent tubes suggests that Texanol is not completely vaporized under these conditions. Water-based lacquers sometimes contain even higher boiling solvents such as dibutyl phthalate (DBP), bp = 340°C, benzyl butyl phthalate, bp = ca. 370°C and di-(2-ethylhexyl) phthalate (DOP), bp = 386°C. A lacquer formulation containing DBP, and neat DOP were investigated according to the following procedure.

Procedure:

A sample weighing 0.5 ± 0.02g was placed in an aluminum weighing dish with a bottom surface area of 19.6 cm^2, containing a paper clip fashioned as a stirrer. A few drops of methanol were added immediately after weighing the sample and the paper clip stirrer was used to coat the bottom of the weighing dish uniformly with the sample. This method gives an approximate wet film thickness (excluding methanol) of 0.2 mm. The methanol was allowed to evaporate at room temperature for 30 minutes and the samples were then placed in a forced air drying oven at 110°C. Samples of the dried paint films (ca. 50-70 mg) were then extracted with 5 mL acetone by sonicating for 30 minutes, diluting with 5 mL methanol containing an internal standard and centrifuging. The supernatant containing the analyte was then gas chromatographed as previously described. DOP was heated as a neat liquid (0.1g) in an aluminum dish and the mass loss was determined by direct weighing.

The results for two coating materials and dioctyl phthalate are shown in Table 13.

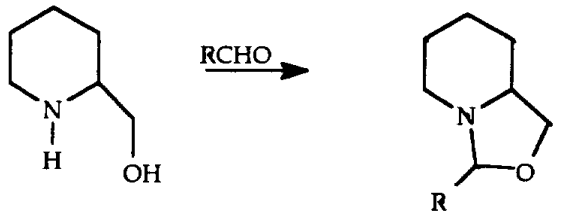
Conclusions

Care must be taken when performing chamber analyses of coatings containing high boiling solvents. The purpose of this portion of the investigation was to identify potential losses of VOCs when sampled at film thicknesses consistent with ASTM 2369. In our subsequent chamber tests, we utilized much thinner films than those described above. These results point out one of the difficulties associated with the term "volatile organic compound". Clearly, some of the solvents used in water-based coatings are not very volatile at all.

F. Investigation of Aldehydes in Coatings

A study was undertaken to determine the significance of aldehydes in selected coating samples. A method for the direct derivatization of aldehydes in latex coatings was developed. The aldehyde content in selected coating samples was determined.

Theory:
Aldehydes react quantitatively with excess 2-hydroxymethylpiperidine (HMP) to give the corresponding oxazolidine derivatives, Equation 1. The lower molecular weight aldehydes, including formaldehyde and acetaldehyde, give stable oxazolidenes which have lower polarities and probably lower boiling points than HMP and can be separated from HMP using a polar chromatography column. Using a Carbowax capillary column, the oxazolidines of formaldehyde (HCHO-OX) and acetaldehyde (CH_3CHO-OX) elute well ahead of the HMP derivatizing reagent.



HMP

R = H, CH_3

Equation 1

Preparation of Standards:
HMP, 0.1983g, and benzonitrile (BN) internal standard, 0.1726g, were dissolved in 10 mL methanol. The mixture was diluted with methanol to give an HMP concentration of 198.3 µg/mL and a BN concentration of 172.6 µg/mL. A 10 mL portion of this solution was treated with excess 37% formaldehyde solution (ca. 40 drops) and let stand for 15 minutes. Gas chromatography showed that all of the HMP was converted to HCHO-OX. The oxazolidine of acetaldehyde, CH_3CHO-OX, was prepared in the same fashion starting with 0.2032g HMP and 0.2198g BN in 10 mL methanol, diluting by a factor of 100 with methanol, and treating 10 mL of the diluted sample with ca. 20 drops of acetaldehyde. After standing for 15 minutes, gas chromatography showed complete conversion of the HMP to CH_3CHO-OX.

Response Factors:
Response factors relative to benzonitrile as internal standard were calculated using the relationship,

RF = (Mass of BN x Area of Analyte)/(Mass of Analyte* x Area of BN)

where Mass of Analyte* = equivalent aldehyde mass calculated from moles of HMP.
Response factors obtained in this fashion were,

HCHO = 3.72
CH_3CHO = 2.82

GC Conditions:
A 30 m x 0.32 mm Carbowax Column was used for the separation. The injection port was maintained at 250°C. The detector, a thermionic nitrogen/phosphorus (NPD), was kept at 270°C. A split injection of 2-3 µL was used. The initial oven temperature was held at 110°C for 6 minutes, then ramped to 230°C at 40°C per minute. The final temperature was held for two minutes.

Table 13 - Solvent Drying Study

WD-23 Semi Gloss Coating Containing 2.9% Texanol

Time, min	% Texanol in film	% of original in film
0	2.90	100.0
40	0.90	43.1%
60	0.70	24.1%
80	0.46	15.9%
100	0.24	8.3%

WD-39 (WC10) Clear Lacquer Containing 2.2% Dibutyl Phthalate

Time, min	% Dibutyl Phthalate in film	% of original left in film
0	2.20	100.0%
40	1.95	88.6%
60	1.86	84.5%
80	1.58	71.8%
100	1.42	64.5%

Neat Dioctyl Phthalate, 100 mg

Time, min	% Dioctyl Phthalate in film
0	100%
30	99.4%
60	98.3%
90	97.7%

Table 14 - Results of Aldehyde Analysis in Selected Coatings

	PPM formaldehyde		PPM acetaldehyde	
sample	average	reported	average	reported
WD02	2	N/A	2	N/A
WD03	0	N/A	2	N/A
WD07	12	N/A	9	N/A
WD09	10	30	134	N/A
WD15	67	30	144	N/A
WD48	0	N/A	58	N/A

Analysis of Paint Samples:
Approximately one gram of latex paint was weighed by difference, to the nearest 0.1 mg, into a solution of 10.0 mL of methanol containing 5 mg/mL of HMP and 50.80 µg/mL of BN in a 15 x 1.5 cm screw-capped test tube. The contents were manually agitated, then sonicated for 10 to 15 minutes and centrifuged. Aliquots of the supernatant liquid were then analyzed by gas chromatography using thermionic detection as described above. A blank containing no paint was also chromatographed. In this study, the blank was found to contain approximately 1.08 µg/mL of formaldehyde and 0.35 µg/mL of acetaldehyde. The source of the blank response was not determined, but it was assumed that it derived from the HMP reagent which was used in its as-received state. The detection limit for both formaldehyde and acetaldehyde using these conditions is approximately 2-3 ppm. The GC retention time for CH_3CHO-OX is 0.5 minutes shorter than the retention time for HCHO-OX with the conditions used for analysis. The possibility that other amines which may be present in the samples might interfere with the analysis was eliminated by comparing GC retention times of some common amines used in the manufacture of latex paints with the retention times of the oxazolidines. These amines included triethyl amine, aminomethyl propanol (AMP-95) and 2-dimethylaminoethanol. The amine AMP-95 (1-amino-2-methyl-2-propanol) also reacts with formaldehyde and acetaldehyde to give oxazolidine derivatives which were not found in the present study.

Rationale for Sample Choices:
- Wd-02, Flat - Vinyl acrylic and could therefore contain residual vinyl acetate hydrolizable to acetaldehyde
- WD-03, 100% acrylic and would therefore not be expected to contain acetaldehyde derived from residual vinyl acetate monomer
- WD-07, Vinyl acrylic and could therefore contain residual vinyl acetate hydrolizable to acetaldehyde
- WD-09, Reported 0.003% formaldehyde on MSDS
- WD-15, - Acrylic enamel, Reported 0.003% formaldehyde on MSDS
- WD-48, Vinyl acrylic and could therefore contain residual vinyl acetate hydrolizable to acetaldehyde

Results:
The results for formaldehyde and acetaldehyde for the six paints which were analyzed are presented in Table 14. In general, the amounts of formaldehyde were quite small in the samples tested. Unexpectedly, more acetaldehyde was found in these paints than formaldehyde. Even in the "worst cases", aldehyde levels were quite low. A small change in the amount of a major component in the sample could easily account for the amount of VOC contributed by aldehydes.

Table 15 - Solvent-based Samples Analyzed by the Direct Method (Solvent Dilution)

sample #	Coating
SD01	Alkyd Enamel
SD02	Polyurethane
SD03	Industrial Enamel, blue
SD04	Industrial Enamel, red
SD05	Industrial Enamel, white
SD06	Industrial Enamel, white
SD07	Polyurethane Enamel
SD08	Polyurethane Catalyst
SD09	Epoxy Curing Agent
SD10	White Epoxy

G. Direct Analysis of Solvent-Based Coating Materials

1. Dilution in Solvent

Since we had some difficulties in obtaining satisfactory results from the chamber samples of solvent-based coatings, due primarily to overloading of the column following thermal desorption of the stainless steel Carbotrap 300 tube, we explored some approaches for the direct analysis of these coating materials. Two approaches proved successful. The simpler approach was a modification of the scheme described earlier, for the direct analysis of water-based coatings. In this method, the sample was diluted with methyl t-butyl ether (MTBE) containing diphenyl methane as internal standard, sonicated, and centrifuged. An aliquot of the MTBE extract was injected onto a 30 meter capillary gas chromatographic column, and the resulting chromatogram analyzed as described previously. This approach worked well for samples containing comparatively few components. Ten samples were analyzed by this technique, as shown in Table 15. The results from these samples will be discussed in a later section.

2. Distillation Procedure

For those samples containing complex solvent mixtures, in particular, mineral spirits, the need for improved resolution of the chromatograms led us to develop an alternate analysis scheme for this class of coating materials. An alternate method of sample preparation, for coatings containing complex, non-polar solvents, was developed and tested. The details of this distillation method are described in this section. The chromatography of these samples was conducted using a 100 meter capillary column (Supelco Petrocol DH, 100m x 0.25 mm).

Procedure

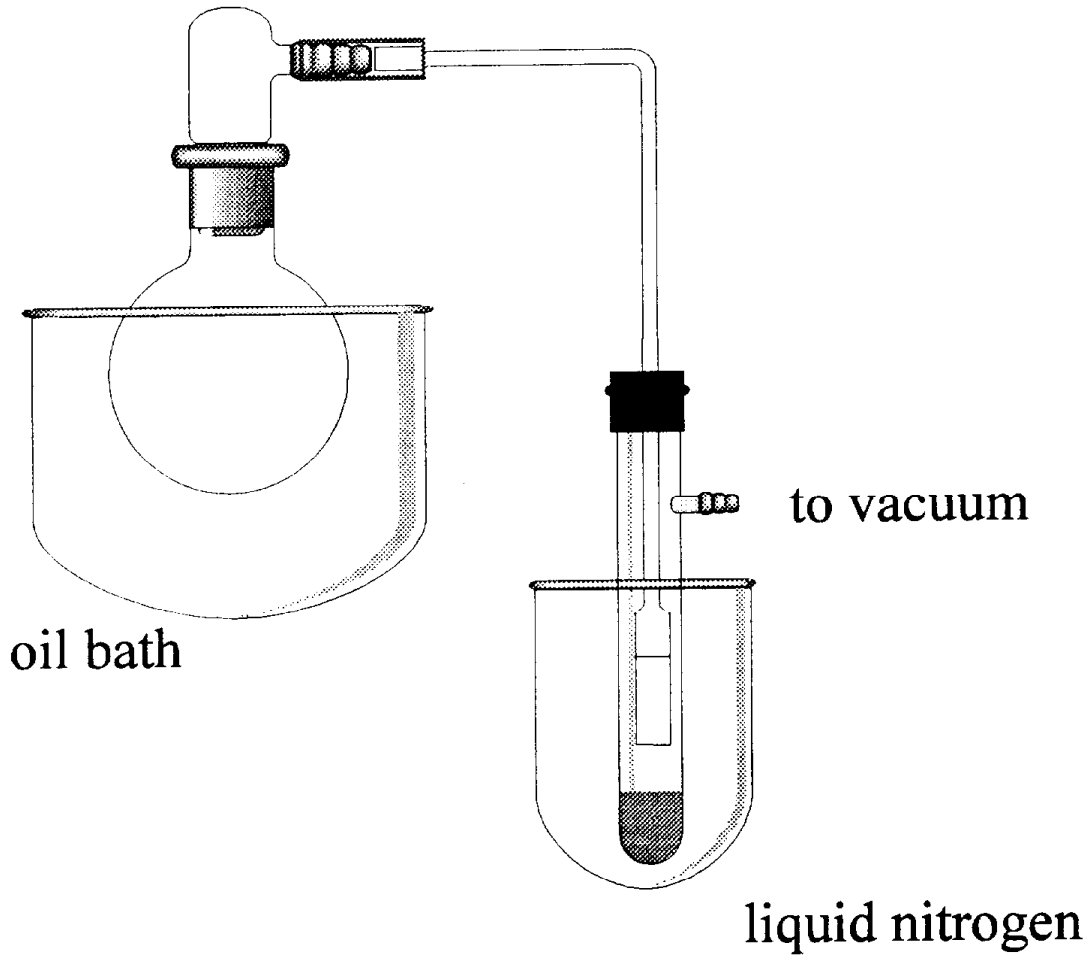
A one to three gram sample of the well mixed paint was added to a 100 mL round-bottom flask containing 5 g of dioctylphthalate (used as a dispersing solvent) and 1.5 g of tetradecane (used as a "chase" solvent). For stains, about 1g of coating was used, while for varnishes and lacquers about 1.5 to 2 g was used. For other paints, about 2 to 3g was used. In general, for low solids-containing paints, a small quantity was used and for high solids-containing paints, a larger amount was used. The mixture was slowly heated in an oil bath, under vacuum, to 120°C and was maintained at 120°C for about 5 to 10 minutes. A schematic diagram of the apparatus is shown in Figure 8.

The pressure was maintained between 0.3 and 0.5 Torr. The distillate was transferred directly to a side arm test tube cooled in liquid nitrogen by means of a piece of glass tubing which was connected directly to the distillation flask and which extended into the collection test tube. At the end of the distillation, the test tube contents were allowed to melt, the test tube was centrifuged, and the contents were transferred to a screw capped vial. The purpose of the dioctyl phthalate was to provide a liquid medium in which the paint was dispersed during the distillation. Since dioctyl phthalate has a boiling point of 380°C, very little (if any) dioctyl phthalate distills with the paint solvents. Since none of the solvent-based paints contained components larger in molecular weight than dodecane (some varnishes contained small amounts of tridecane), the addition of tetradecane to the distillation mixture made it possible to distill the original paint solvents completely out of the paint. The difference in boiling point between dodecane, usually the highest boiling solvent in paint and present in very low concentrations, and tetradecane is 40 Celsius degrees. Thus when tetradecane began distilling, the last traces of the original paint solvents were also distilled out and collected with the tetradecane distillate.

Table 16 - Components of Synthetic 42 Component Standard

Pk#	RI, Exptl	Ret Time, min.	Compound
1	400.0	14.230	Methanol
2	467.8	16.728	Acetone
3	500.0	17.917	Pentane
4	528.4	19.822	2,2-Dimethylbutane
5	562.2	22.021	2-Methylpentane
6	569.6	22.498	MEK
7	579.1	23.118	3-Methylpentane
8	600.0	24.479	Hexane
9	658.7	30.285	Cyclohexane
10	663.7	30.786	MPK
11	674.6	31.862	3-Methylhexane
12	689.7	33.353	2,2,4-Trimethylpentane
13	700.0	34.374	Heptane
14	723.3	36.852	Methylcyclohexane
15	756.9	40.433	Toluene
16	779.9	42.877	cis-1,3-Dimethyl CH
17	781.8	43.082	trans-1,4-Dimethyl CH
	797.9	44.799	trans 1,2-DiMe CH
18	800.0	45.021	Octane
19	806.9	45.705	trans-1,3 DiMe CH
	806.9	45.705	cis-1,4 DiMe CH
20	832.1	48.185	cis 1,2-DiMe CH
21	834.6	48.428	Chlorobenzene
22	853.5	50.297	Ethylbenzene
23	862.9	51.227	p-Xylene
24	885.1	53.413	o-Xylene
25	900.0	54.88	Nonane
26	917.9	56.467	isoPropylbenzene
27	963.2	60.474	1,3,5-Trimethylbenzene
28	989.0	62.765	1,2,4-Trimethylbenzene
29	1000.0	63.737	Decane
30	1020.6	65.4	p-Cymene
31	1033.0	66.405	Indan
32	1051.6	67.912	p-Diethylbenzene
33	1053.1	68.03	Butylbenzene
34	1070.4	69.427	trans-Decalin
35	1100.0	71.824	Undecane
36	1116.2	73.053	cis-Decalin
37	1155.0	76.005	Amylbenzene
38	1187.3	78.461	Naphthalene
39	1200.0	79.426	Dodecane
40	1300.0	86.81	Tridecane
41	1303.7	87.093	2-Methylnapthalene
42	1400.0	94.451	Tetradecane

Figure 8 - Diagram of Solvent Distillation Apparatus



Assignment of Linear Retention Indices

The linear retention indices were assigned using a combination of techniques. Peaks for the linear n-alkanes were easily identified from the chromatograms and retention indices (RI) for these were assigned in the usual manner (retention index = 100 x C_n). Experimental linear retention indices (RI) were then calculated for all peaks in both the GC/FID (100 m) and GC/MS (30 mm for all and 100 m for selected samples) chromatograms, using the equation:

$$RI = 100n + 100\frac{t_r(component) - t_r(C_n)}{t_r(C_{n+1}) - t_r(C_n)}$$

where t_r values are the retention times for the sample component, and the normal hydrocarbons whose retention times bracket the sample peak. Several known alkane, cycloalkane, aromatic, and oxygenated standard samples were run and their retention indices determined. Calibration values supplied with the 100 m column were used to obtain initial estimates of other indices. For further information on retention indices, the reader is directed to the literature. Two pertinent references are:

1. Khorasheh, Gray and Selucky, *J. Chromatog.*, 481 (1989) 1-16
2. Hayes and Pitzer, *J. Chromatog.*, 253 (1982) 179-198.

Primary assignments were obtained from the standard values determined as noted above, and from the mass spectrometric identifications of the peaks in the chromatograms. Over twenty samples were initially evaluated and their retention indices compared with one another and with the published and standard indices to insure accurate assignments. A compilation of retention indices for the 100 meter column was prepared and used in the identification of further samples. For peaks with uncertain or unknown identification, a determination was first made as to whether the peak was due to an oxygenated or aromatic compound. The presence or absence of alkyl aromatic compounds could be determined easily by examining the relevant mass spectra, and checking for the presence of ions of large abundance having m/e of 77 or 91. Figure 9 shows an extracted ion chromatogram of m/e = 91 overlaid with a region of a chromatogram for sample SD33. The identity of alkyl aromatic peaks becomes immediately apparent. All oxygenated and aromatic peaks could be identified and assigned without ambiguity. If an unknown peak was shown to be neither an oxygenate nor aromatic, the peak was classified as a "C_n" peak if its retention time was greater than that for the linear alkane C(n-1) and less than that for C_n. For example, an unidentified peak with a retention index of 1050 would be assigned as C11.

In all cases, over 90% of the total VOCs (based on integrated areas of all peaks) could be identified, with the majority of samples having over 95% of the VOC speciated.

Validation

A sample of 2.981g of paint (SD56), which was known to contain no benzene, chlorobenzene, or tridecane was spiked with 167.6 mg of a mixture of these three substances. The composition of the mixture was 16.13% benzene, 65.00% chlorobenzene, and 18.87% tridecane. The spiked paint was distilled as described above and the distillate was chromatographed on a 100m x 0.25 mm capillary column. In a separate experiment, a different paint (SD52, a Satin Varnish), also known not to contain the spike mixture components, was subjected to the distillation procedure and the distillate was then spiked with 152.6 mg of the same spike mixture used for SD56. The ratio of the chromatographic peak areas, normalized to chlorobenzene at 100, was then measured for each sample. The results are presented below.

	Benzene	Chlorobenzene	Tridecane
SD56	32.15	100	36.40
SD52	32.84	100	38.45

Benzene was chosen as an analyte which might have been lost because of its relatively low boiling point while tridecane might have been recovered in less than the spike amount for SD56 because of its relatively high boiling point. Chlorobenzene has an intermediate boiling point and was assumed that recovery for it should be 100%. Since the ratios were approximately the same for the two samples it was concluded that all of the paint solvents were distilled out of the mixture and that all of the solvents were recovered quantitatively.

3. Analysis Methods

The solvent-based coating samples prepared by distillation were analyzed on a 100 meter x 0.25 mm capillary column (Supelco Petrocol). Initial runs were made using a flame ionization detector. For many of the samples, more than 100 resolved peaks were obtained. Many of these peaks could be identified by means of a retention index library, supplied by the column manufacturer. However, some peaks had indices which did not correspond to any in the index library. In order to identify these components, we ran the sample extracts on a 30 meter x 0.25 mm HP-5 capillary column, in a Hewlett Packard Series II Gas Chromatograph equipped with a mass spectral detector (G1800). The resulting peaks were searched against a NIST mass spectral library. This procedure resulted in positive identifications for nearly all sample peaks. For samples with complex chromatograms, we re-ran them, mounting the same 100 meter capillary column used for the GC-FID analyses into the GC-MS system. We developed a correlation expression that enabled us to update the retention index library with the components identified by the mass spectrometric detector.

IV. Results

A. Water-Based Coatings

1. Direct Analyses

Using the direct methods described earlier (Section III.E, pages 28-30), emission profiles were obtained for 52 water-based coating samples. Table 17 shows the nature of the coating samples analyzed. In all cases, the species profiles were obtained by averaging the results of at least two analyses. Typical agreement for replicates was good, with standard deviations on the order of three or four percent, relative to the mean. Table 18 shows sample statistics for sample WD05. Appendix B shows the emission profiles for all water-based coating samples analyzed. A total of twenty-four different solvents was found in these samples. The distribution of solvents found in the water-based samples tested is shown in Table 19. The four most common solvents were identified as Texanol (found in 37/52 of the coatings), propylene glycol (31/52), diethylene glycol butyl ether (23/52), and ethylene glycol(14/52). The solvent systems used in these coatings were fairly simple. As is shown in Figure 10, a binary component solvent system was common, with 23 out of 52 coatings falling into this description. The identification rate of chromatography peaks for these samples was high. In all but 4 samples, 100% of the VOC mass was positively identified. For the other four samples, a carbon number was assigned, based on the retention index of the minor unknown peak(s).

Sample WD36 was found to contain glycerin as a major VOC component (about 85% of the total VOC). This was the only sample in which glycerin was present. It was felt that incorporating the species profile from this sample into a group profile (Group 6w) would produce a non-representative species profile for the group, showing an "average" sample as containing glycerin, while this was the exception to coatings in this category. The species profile for sample WD36 is shown in Appendix A, along with the other water-based coating samples.

2. Chamber Analyses

Using the methods described earlier, several chamber tests were made. Emissions from the selected coating samples were collected on ORBO100 tubes, which were solvent extracted, then analyzed by GC-FID. Comparisons for a water-based coating sample, analyzed by the direct and chamber methods, are shown in Table 20. The overall agreement of the species profiles by both methods is good, with variations of a few percent between the two methods. The results of another comparison of chamber and direct determinations are shown in Table 21. This sample, a two component water-reducible lacquer containing dibutyl phthalate and 2-butoxyethanol, was described earlier in this report. As Table 21 shows, agreement for 2-butoxyethanol by the two methods is excellent (3% relative variation). The dibutyl phthalate was under-determined by the chamber method, not surprising, based on the boiling point of 370°C for dibutyl phthalate. Refer again to Table 13 to see the time dependence of the loss of dibutyl phthalate from coating samples. Under the chamber conditions used (110°C for 1 hour), more than three-fourths of the dibutyl phthalate remained associated with the paint film. For components of "ordinary" volatility, the chamber method provided results consistent with the direct method. For components with very low volatility, the chamber method produced results that were systematically low, relative to the direct method.

Figure 9 - Identification of Aromatic Peaks in Sample SD33

Upper trace: m/e 91 abundance; lower trace, Total Ion Chromatogram

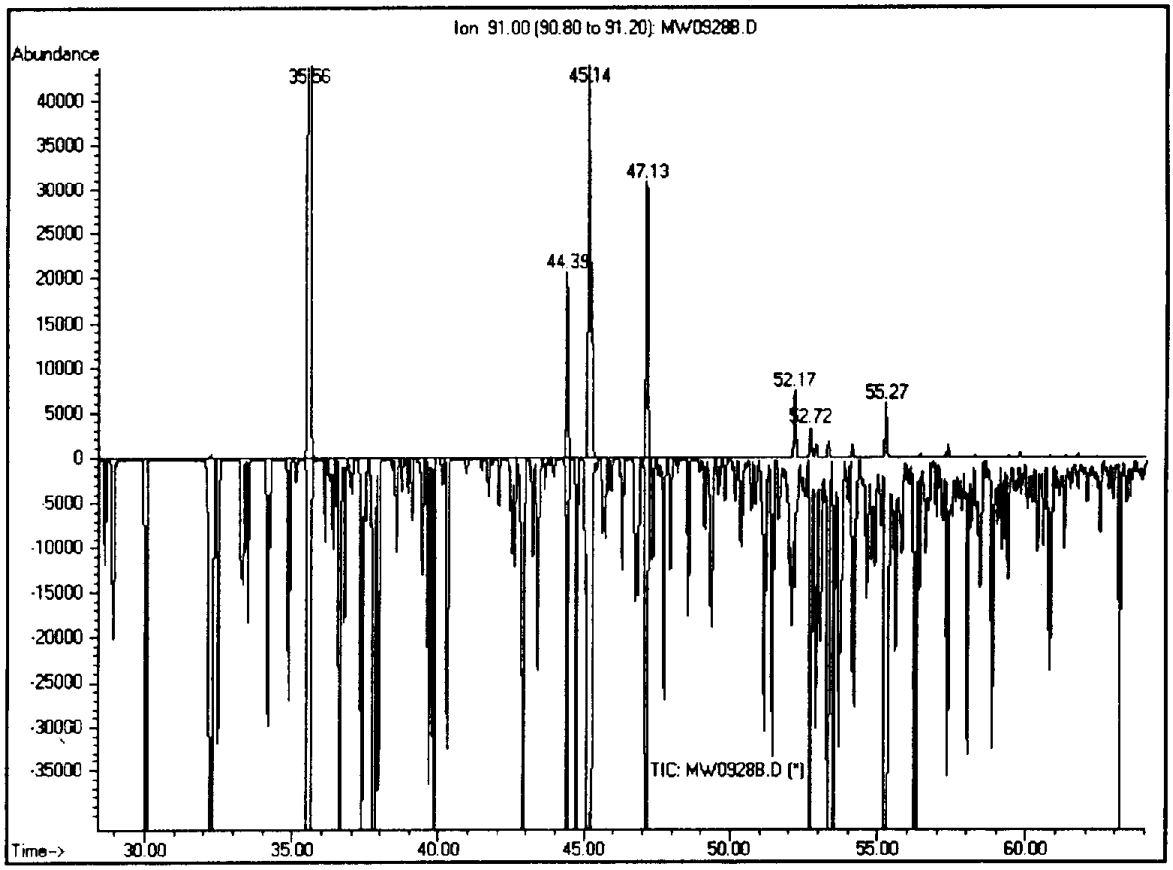


Table 18 - Statistics for Replicate Runs, Sample WD-05

Sample WD05- Semi-Gloss Latex

	WD05a1	WD05a2	WD05b1	WD05b2	WD05c1	WD05c2	Average	sigma	wt. fraction
% PG	3.61	3.65	3.47	3.46	3.74	3.80	3.62	0.14	0.7973
% TX	0.87	0.89	0.93	0.90	0.97	0.97	0.92	0.04	0.2027
TOTAL							4.54		1.0000

Table 17 - Water-Based Samples Analyzed by the Direct Method

sample	Coating type
WD01	Lo Gloss
WD02	Flat
WD03	Gloss
WD04	Semi Gloss
WD05	Lo Gloss
WD06	Semi Gloss
WD07	Semi Gloss
WD08	stain
WD09	Vinyl Acrylic Flat
WD10	Lo Gloss Latex Latex
WD11	Lo Gloss Latex
WD12	Semi Gloss Latex
WD13	Gloss
WD14	Stain
WD15	Acrylic Semi-Gloss
WD16	Acrylic Flat
WD17	varnish
WD18	clear varnish
WD19	Clear Gloss
WD20	Wood Stain
WD21	Flat
WD22	Lo Gloss
WD23	Semi Gloss
WD24	Semi Gloss Latex
WD25	Flat
WD26	Lo Gloss
WD27	Acrylic Hi Gloss
WD28	Latex Flat, White
WD29	Acrylic Flat
WD30	Latex Semi Gloss
WD31	Flat
WD32	Lo Gloss
WD33	Semi Gloss
WD34	Semi Gloss
WD35	Flat
WD36	Stain
WD37	Traffic
WD38	Traffic
WD39	Water Reducible Lacquer
WD40	Sanding Sealer
WD41	Acrylic Traffic
WD42	Latex Traffic
WD43	Traffic Paint
WD44	Traffic Paint
WD45	Water Reducible Stain
WD46	Gloss
WD47	Flat
WD48	Lo Gloss
WD49	Semi Gloss
WD50	Lo Gloss
WD51	Semi Gloss
WD52	Flat

Figure 10 - Distribution of Solvents in Water-Based Coating Samples

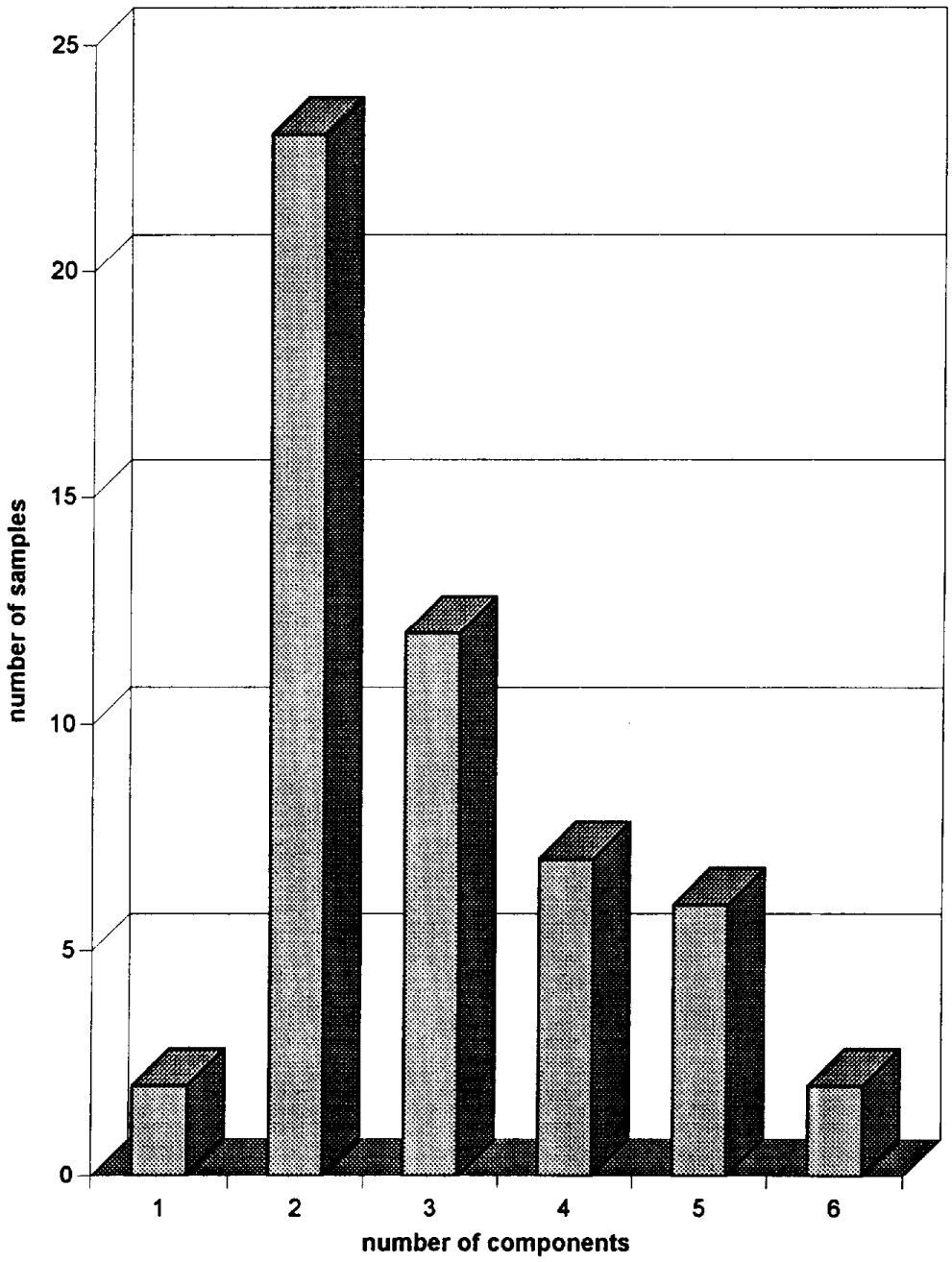


Table 19 - Distribution of Solvents in Water-Based Coating Samples

Component	present in samples
Texanol	37
propylene glycol	31
diethylene glycol butyl ether	23
ethylene glycol	14
2-butoxyethanol	7
isopropyl alcohol	5
methanol	5
N-methylpyrrolidone	4
unknown	4
dipropylene glycol methyl ether	3
dibutyl phthalate	2
diethylene glycol methyl ether	2
ethanol	2
1-butoxy-2-propanol	2
sec-butyl alcohol	2
1-amino-2-methyl-2-propanol	2
diethylene glycol ethyl ether	1
diethylene glycol	1
dipropylene glycol butyl ether	1
glycerin	1
hexylene glycol	1
methyl amyl ketone	1
2-methoxy-1-propanol	1
1-propoxy-2-propanol	1

Table 21 - Comparison of Chamber and Direct Analyses for a Water-Reducible Lacquer

	% composition		
	WC10	WD39	RATIO
	average chamber	average direct	chamber/ direct
component			
2-butoxyethanol	9.17	9.44	0.97
dibutyl phthalate	0.20	0.92	0.21

Table 20 - Comparison of Chamber and Direct Low Gloss Latex Enamel Profiles

Comparison of WC07 and WD11

	emission profile		RATIO
	WC07	WD11	chamber/direct
component	chamber	direct	
propylene glycol	0.4588	0.4457	1.03
diethylene glycol butyl ether	0.0677	0.0690	0.98
Texanol	0.4735	0.4852	0.98

2. Chamber Analyses

Using the methods described earlier, a number of chamber tests were made. In the first of these tests, a coating sample for which a successful direct analysis had been conducted was selected. Emissions from this coating were collected on Carbotrap 300 stainless steel sorbent tubes. When analyzed by thermal desorption into a GC-FID system, unacceptable resolution and low identification rates were obtained for the major components in the sample. Eventually, this was attributed to the relatively high VOC loading of the sorbent tube. The project subcontractor prepared a modification of his chromatographic inlet system that allowed for the splitting of the effluent from the sorbent tube following thermal desorption. This system resulted in much improved chromatography, but peak widths and shapes were still inferior to those obtained by direct analysis. In such complex samples, the extra broadening introduced by the thermal desorption process was enough to preclude the satisfactory resolution of closely eluting sample components. No satisfactory profiles were obtained using thermal desorption of the chamber emissions collected on Carbotrap 300 sorbent tubes.

A comparative study of the two previously described sorbent tube types was performed. The chamber sampling manifold was modified to allow two steel Carbotrap 300 tubes to be used simultaneously with one glass Carbotrap 100 tube. The analysis of the steel tubes by thermal desorption showed a loss of material above the C10 range of the chromatogram, relative to the direct analysis. No such loss was observed in the solvent extracted ORBO tube. This demonstrated that the solvent vapors emitted during the drying process were transferred efficiently to the sorbent tubes. The higher molecular weight components apparently were not efficiently transported to the GC column by the thermal desorption process.

In a final chamber test, the emissions from a Redwood stain coating sample were collected on two ORBO100 tubes, which were solvent extracted, then analyzed by GC-FID. Results from these analyses (chamber test SC15 and direct analysis SD55) are shown in Table 23. This table contains data from duplicate direct and duplicate chamber analyses. To illustrate the variability, results from the first run were divided by the second run. For perfect agreement, the entries of the ratio columns should all equal 1.000. Over the 128 peaks found in the chromatogram for this sample, variations between duplicate direct runs produced an average ratio of 1.083. If the comparison is restricted to those 26 peaks corresponding to components in excess of 0.50 % (26 of these accounted for about 80% of the total VOC), the average ratio was seen to be 1.002.

A similar analysis was performed for the duplicate chamber runs. As Table 23 shows, the variation between runs is comparable to that obtained for the direct runs (1.086 vs. 1.083). However, agreement for the minor components is more variable than in the direct runs. This is to be expected, since the amount of material collected during the chamber runs results in a lower concentration of VOCs being presented to the gas chromatograph, producing more uncertainty in the integration of peaks, which is most apparent for the minor components (<0.50% of the Total VOC). If the comparison is again restricted to the 26 largest components, the relative variation between chamber runs produces a ratio of 1.127 (12 % variation). The agreement of the species profiles for major components by both methods is good. The direct method allows for improved speciation of the minor components.

B. Solvent-Based Coatings

1. Direct Analyses

Using the methods described earlier (see pages 41 and 45), emission profiles were obtained for 54 solvent-based coating samples. Table 22 shows the nature of the coating samples analyzed. Samples SD01 through SD10 were analyzed using the direct, solvent dilution method. Samples SD11 though SD54 were analyzed using the distillation procedure described earlier. The quantitative components of the species profiles were obtained from the GC-FID runs. Each of the solvent-based coating samples was analyzed both by GC-FID and by GC-MS. The GC-MS information was used to aid in the identification of peaks, as described earlier. The agreement for replicates was good, with variations on the order of a few percent relative. Table 23 shows this for sample SD-55. Emission profiles for all solvent-based coating samples analyzed are shown in Appendix C. Each sample was analyzed individually, with no *a priori* set list of target compounds. All chromatographic peaks were reported and analyzed for all samples. The sample-to-sample variation in composition produced profiles with varying numbers of components, as shown in Appendix C. Since various petroleum fractions were used in these solvent-based coatings, complex mixtures of various isomers of aliphatic and aromatic hydrocarbons accounted for the diversity of chromatographic peaks observed. A typical chromatogram for one such sample is shown in Figure 11. The upper part of this figure identifies major peaks obtained using the GC-FID, while the lower portion shows the same sample analyzed using the GC-MS system. In contrast to the simple systems seen with the water-based coatings, the solvent-based systems contained up to several hundred components.

D. Comparison of Analytical Results with MSDS

In order to asses the quality of information provided by existing literature sources, a number of comparisons were made between analytical results obtained in our laboratory, and information available on the Material Safety Data Sheets and Product Data Sheets for a number of coating samples.

The MSDS was intended primarily as an aid to the safe handling and use of the material. Sufficient information is usually presented to assess the health risk, and provide guidelines to fire fighters who may be faced with the material in question. Many MSDS indicate "less than.." amounts for reporting concentrations below some regulatory or health limit. Some of the MSDS we examined contained only the statement: "NO OSHA HAZARDOUS INGREDIENTS OVER 1%". In other cases, the identity of the components present in the material was reported, but amounts would not be reported, still satisfying the reporting requirements of Title III and 40 CFR 372. In many cases, composition information was reported as % of a generic solvent (*e.g.*, mineral spirits). As we have shown, these solvents may have several hundred components.

1. Water-Based Coating Samples

During the analysis of these coating samples, quantitative composition information was generated, which could be converted into VOC content, in grams per liter. A comparison of manufacturer-provided VOC content with those calculated from our results is shown in Table 26. In general, the agreement between calculated and reported was good, with an average variation of 4%. As Figure 12 shows, there were more cases in which the calculated values were larger than reported.

In addition to the VOC content, the actual species reported on the MSDS were compared with those found by our analysis. These comparisons are detailed in Appendix B. There were cases in which components exceeding 1 % as determined by direct analysis were not reported on the MSDS.

2. Solvent-Based Coating Samples

For these samples, species profiles were generated which were based on the total of all VOC species found by GC analysis. These relative values do not allow the calculation of absolute VOC content of the samples, so comparisons like those reported for the water-based samples are not possible.

The comparison of listed species is more complicated than with the water-based paints, because of the large number of components present in many solvent-based coatings, and because of the tendency to report generic solvent mixtures, rather than individual chemical species. With these constraints, we examined our results for the solvent-based coating samples, and compared them with MSDS information. Table 27 shows the results of these comparisons. It shows samples for which species were identified by GC analysis, at levels of 1% or greater, but not reported on the MSDS.

Conclusions

For most coatings studies, the VOC measured by our analyses were consistent with the reported VOC values. The agreement of our species profiles with the list of components in the MSDS were less than perfect. In many instances, the MSDS failed to indicate species identified by direct analysis of the coating samples; in other cases, the amounts of materials were over- or understated.

C. Composite Emission Profiles

As described in the beginning of this report, coatings were initially assigned into one of eleven working groups. Table 24 shows the composition of each group. A composite emission profile was constructed for each class, by summing all the fractional components for all samples in the profile, and normalizing the sum to exactly 1.00. By this process, those components that were found in few samples were given less weight than those present in a larger number of samples. It is important to keep in mind that these group profiles reflect a composite of profiles from all coatings analyzed in a given class. As the finished profiles were evaluated, it became apparent that additional sub-classes would be needed. For groups 2, 6, and 7, sub-groups corresponding to carrier technologies were developed. Thus, Group 2s contains the composite profile for solvent-based coatings, and Group 2w contains the composite profile for water-based coatings. Groups 6s, 6w, 7s, and 7w are similarly defined. Composite species profiles for these groups are shown in Appendix D. The number of components in these profiles ranges from 100 to over 300. Many of the identified components are present in very small overall fractions. Table 25 shows the number of components required to account for 50, 75, 90, and 100 % of the total speciated VOC mass.

Figure 11 - Chromatogram of Solvent-Based Coating, Direct Method

GC-FID upper trace; GC-MS lower trace

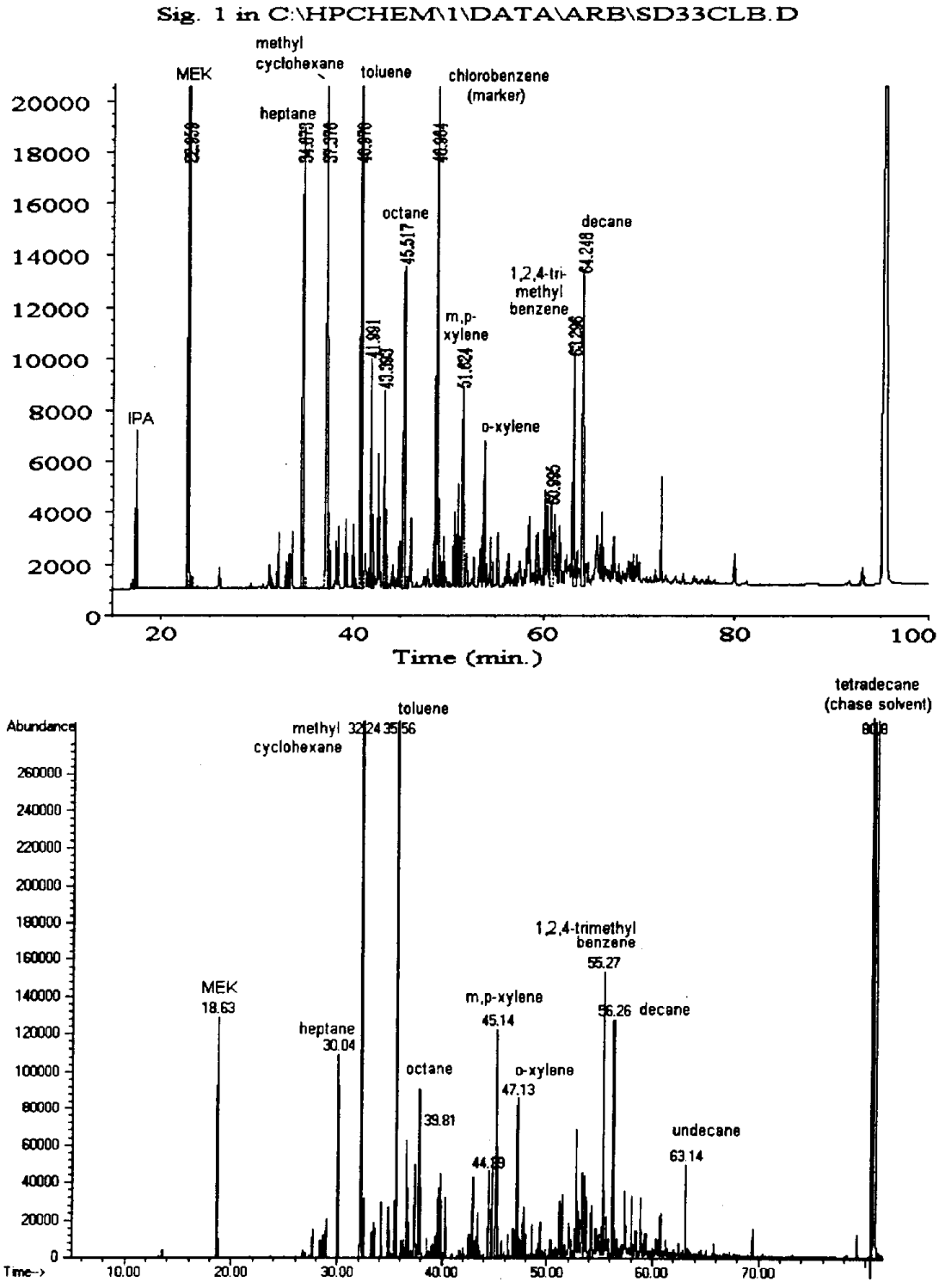


Table 22 - Solvent -Based Samples Analyzed by the Direct Method

SD01	Gloss Enamel
SD02	Polyurethane
SD03	Industrial Enamel
SD04	Industrial Enamel
SD05	Industrial Enamel
SD06	Industrial Enamel
SD07	Polyurethane Enamel
SD08	Polyurethane Catalyst
SD09	Epoxy Curing Agent
SD10	White Epoxy
SD11	Stain Blocking Primer
SD12	Gloss White
SD13	Industrial Maintenance
SD14	Lacquer Diluent
SD15	Lacquer Thinner
SD16	Commercial Mineral Spirits
SD17	Gloss Alkyd
SD18	White Industrial Maint. Enamel
SD19	VM&P Naptha
SD21	Mineral Spirits
SD22	Semi-Gloss
SD23	Alkyd Gloss
SD24	Semi-Gloss Alkyd
SD25	High Gloss Industrial Enamel
SD26	Spar Varnish
SD27	Clear gloss polyurethane
SD28	White Lacquer
SD29	Quick-Dry Alkyd Gloss Enamel
SD30	Yellow Epoxy Primer
SD31	Polyurethane Enamel
SD32	White Industrial Coating
SD33	Industrial Red Oxide Primer
SD34	Epoxy
SD35	Epoxy Converter
SD36	Sanding Sealer Lacquer
SD37	Clear Lacquer
SD38	Clear Wood Finish
SD39	Alkyd Traffic Paint
SD40	Alkyd Semi-Gloss
SD41	Alkyd Gloss
SD42	Alkyd Semi-Gloss
SD43	Oil-Base Semi-Gloss
SD44	Primer
SD45	Primer
SD46	Enamel Undercoat
SD47	Wood Primer
SD48	Sign Painter's Lettering Enamel
SD49	Graphic Arts Coating, Blue
SD50	Varnish
SD51	Clear Varnish
SD52	Clear Satin Varnish
SD53	Semi-Transparent Stain
SD54	Semi-Transparent Stain
SD55	Redwood Stain

Note: Samples SD01-10 analyzed by solvent dilution GC; balance of samples analyzed by distillation

Table 23 - Comparison of Chamber and Direct Solvent-Based Redwood Stain Profiles

	DIRECT ANALYSIS					CHAMBER ANALYSIS				
		#1	#2	Avg. #1, #2	#1/#2	#3	#4	Avg. #3, #4	#3/#4	Avg direct/ avg.chamber
Pk#	Compound	Area %	Area %			Area %	Area %			
68	methyl propylcyclohexane	0.225	0.215	0.220	1.05	0.184	0.14	0.16	1.31	1.36
69	indane	0.946	0.965	0.955	0.98	0.894	0.516	0.71	1.73	1.36
70	isobutylcyclohexane	0.159	0.197	0.178	0.81	0.065	0	0.03		5.48
71	butylcyclohexane	0.208	0	0.104		0.07	0.045	0.06	1.56	1.81
72	pentylcyclopentane	0.465	0.46	0.463	1.01	0.306	0.278	0.29	1.10	1.58
73	3,7-dimethylnonane	0.280	0.287	0.284	0.98	0.19	0.162	0.18	1.17	1.61
74	1,3-diethylbenzene	0.416	0.412	0.414	1.01	0.323	0.281	0.30	1.15	1.37
75	1-methyl-3-propylbenzene	0.867	0.882	0.874	0.98	0.758	0.696	0.73	1.09	1.20
76	1,3-dimethyl-5-ethylbenzene	1.705	1.662	1.684	1.03	1.575	1.312	1.44	1.20	1.17
77	5-methyldecane	0.461	0.31	0.386	1.49	0.329	0.238	0.28	1.38	1.36
78	4-methyldecane	0.164	0.143	0.154	1.15	0.218	0.145	0.18	1.50	0.85
79	1-methyl-2-propylbenzene	0.330	0.326	0.328	1.01	0.385	0.271	0.33	1.42	1.00
80	trans-decalin	0.143	0.129	0.136	1.11	0.208	0.31	0.26	0.67	0.53
81	3-methyldecane	0.581	0.577	0.579	1.01	0.753	0.507	0.63	1.49	0.92
82	1,4-dimethyl-2-ethylbenzene	0.685	0.705	0.695	0.97	0.519	0.367	0.44	1.41	1.57
83	1,3-dimethyl-4-ethylbenzene	0.326	0.322	0.324	1.01	0.267	0.177	0.22	1.51	1.46
84	1,1-dimethyl-2-propylcyclohex	0.176	0.153	0.165	1.15	0.139	0.105	0.12	1.32	1.35
85	1,2-dimethyl-4-ethylbenzene	0.699	0.7	0.700	1.00	0.579	0.495	0.54	1.17	1.30
86	1,3-dimethyl-2-ethylbenzene	0.152	0.138	0.145	1.10	0.06	0.057	0.06	1.05	2.48
87	ethyl propylcyclohexane	0.093	0.077	0.085	1.21	0.097	0.085	0.09	1.14	0.93
88	cis-decalin	0.653	0.657	0.655	0.99	0.584	0.473	0.53	1.23	1.24
89	ethyl propylcyclohexane	0.069	0	0.035		0	0.05	0.03	0.00	1.38
90	OTHER C11	0.077	0	0.039		0	0.125	0.06	0.00	0.62
91	ethyl propylcyclohexane	0.181	0.154	0.168	1.18	0	0	0.00		
92	undecane	0.736	0.733	0.735	1.00	0.836	0.572	0.70	1.46	1.04
93	2-methyldecalin	0.391	0.435	0.413	0.90	0.314	0.161	0.24	1.95	1.74
94	OTHER C12	0.168	0.2	0.184	0.84	0.203	0.108	0.16	1.88	1.18
95	1,2,4,5-tetramethylbenzene	0.200	0.208	0.204	0.96	0.181	0.097	0.14	1.87	1.47
96	1,2,3,5-tetramethylbenzene	0.419	0.444	0.432	0.94	0.268	0.219	0.24	1.22	1.77
97	2-methyldecalin	0.169	0.153	0.161	1.11	0.24	0.168	0.20	1.43	0.79
98	1,3-dimethyl-4-isopropylbenze	1.076	1.063	1.069	1.01	1.069	0.906	0.99	1.18	1.08
99	(2-methylbutyl)cyclohexane	0.119	0.047	0.083	2.53	0.038	0.031	0.03	1.23	2.41
100	5-methylindane	0.210	0.231	0.221	0.91	0		0.00	0.00	
101	hexylcyclopentane	0.152	0	0.076		0.18	0.165	0.17	1.09	0.44
102	pentylcyclohexane	0.638	0.608	0.623	1.05	0.328	0.398	0.36	0.82	1.72
103	4-methylindane	0.552	0.478	0.515	1.16	0.366	0.362	0.36	1.01	1.42
104	1,2,3,4-tetramethylbenzene	0.223	0	0.112		0.116	0.181	0.15	0.64	0.75
105	4-ethyldecane	0.540	0.492	0.516	1.10	0.491	0.422	0.46	1.16	1.13
106	5-methylundecane	0.158	0.123	0.141	1.29	0.203	0.234	0.22	0.87	0.64
107	4-methylundecane	0.178	0.126	0.152	1.41	0	0	0.00		
108	OTHER C12	0.108	0.098	0.103	1.10	0	0	0.00		
109	2-methylundecane	0.329	0.272	0.301	1.21	0.195	0.238	0.22	0.82	1.39
110	3-methylundecane	0.581	0.449	0.515	1.29	0.334	0.328	0.33	1.02	1.56
111	OTHER C12	0.165	0.088	0.127	1.88	0.139	0.078	0.11	1.78	1.17
112	methyl pentylcyclohexane	0.128	0.066	0.097	1.94	0.056	0.049	0.05	1.14	1.85
113	naphthalene	0.486	0.347	0.417	1.40	0.31	0.254	0.28	1.22	1.48
114	5,6-dimethylindane	0.493	0.463	0.478	1.07	0.377	0.374	0.38	1.01	1.27
115	dodecane	0.581	0.563	0.572	1.03	0.48	0.452	0.47	1.06	1.23
116	OTHER C13	0.467	0.545	0.506	0.86	0.474	0.468	0.47	1.01	1.07
117	1,3,5-triethylbenzene	0.254	0.171	0.213	1.49	0.19	0.182	0.19	1.04	1.14
118	1,1,5-trimethylindane	0.296	0.235	0.266	1.26	0.265	0.213	0.24	1.24	1.11
119	2,6-dimethylundecane	0.252	0.206	0.229	1.22	0.221	0.169	0.20	1.31	1.17
120	3,6-dimethylundecane	0.140	0.096	0.118	1.46	0.155	0.106	0.13	1.46	0.90
121	2,7-dimethylundecane	0.250	0.18	0.215	1.39	0.146	0.137	0.14	1.07	1.52
122	OTHER C13	0.054	0	0.027		0.076	0.133	0.10	0.57	0.26
123	hexylcyclohexane	0.107	0.062	0.085	1.73	0.129	0.128	0.13	1.01	0.66
124	2,9-dimethylundecane	0.264	0.211	0.238	1.25	0.276	0.305	0.29	0.90	0.82
125	4,7-dimethylindane	0.110	0.089	0.100	1.24	0.075	0.062	0.07	1.21	1.45
126	2,10-dimethylundecane	0.072	0.083	0.078	0.87	0.091	0.041	0.07	2.22	1.17
127	OTHER C13	0.157	0.152	0.155	1.03	0.172	0.165	0.17	1.04	0.92
128	tridecane	0.247	0.24	0.244	1.03	0.312	0.3	0.31	1.04	0.80
	Fraction Identified									
128	all peaks	100.00	100.00	99.62	1.083	98.36	97.64	98.00	1.086	1.183
26	peaks>0.5%			78.27	1.002			78.54	1.078	1.127

Table 23 - Comparison of Chamber and Direct Solvent-Based Redwood Stain Profiles

SD55, Redwood Stain		Distillation				Chamber Run SC15				
	DIRECT ANALYSIS					CHAMBER ANALYSIS				
		#1	#2	Avg. #1, #2	#1/#2	#3	#4	Avg. #3, #4	#3/#4	Avg direct/ avg.chamber
Pk#	Compound	Area %	Area %			Area %	Area %			
1	methylcyclohexane	0.062	0.06	0.061	1.03	*0.229*	*0.358*	*0.29*	*0.64*	*0.21*
2	toluene	0.057	0.06	0.059	0.95	*0.217*	*0.316*	*0.27*	*0.69*	*0.22*
3	2-methylheptane	0.059	0.065	0.062	0.91	0.071	0.088	0.08	0.81	0.78
4	cis-1,3-dimethylcyclohexane	0.152	0.144	0.148	1.06	0.145	0.192	0.17	0.76	0.88
5	trans-1,4-dimethylcyclohexane	0.053	0.05	0.052	1.06	0.119	0.053	0.09	2.25	0.60
6	octane	0.211	0.224	0.218	0.94	0.249	0.302	0.28	0.82	0.79
7	cis-1,4-dimethylcyclohexane	0.077	0.087	0.082	0.89	0.09	0.104	0.10	0.87	0.85
8	2,6-dimethylheptane	0.142	0.14	0.141	1.01	0.085	0.108	0.10	0.79	1.46
9	2,7-dimethylheptane	0.087	0	0.044		0.087	0.144	0.12	0.60	0.38
10	ethylcyclohexane	0.117	0.205	0.161	0.57	0.147	0.141	0.14	1.04	1.12
11	1,1,3-trimethylcyclohexane	0.258	0.279	0.269	0.93	0.265	0.353	0.31	0.75	0.87
12	OTHER C9	0.067	0.097	0.082	0.69	0.052	0.054	0.05	0.96	1.55
13	OTHER C9	0.056	0.062	0.059	0.90	0.027	0.057	0.04	0.47	1.41
14	ethylbenzene	0.374	0.391	0.383	0.96	0.416	0.579	0.50	0.72	0.77
15	trans, trans-1,2,4-trimethylcycl	0.281	0.293	0.287	0.96	0.268	0.368	0.32	0.73	0.90
16	2,3-dimethylheptane	0.117	0	0.059		0.064	0.043	0.05	1.49	1.09
17	m-xylene	0.941	0.922	0.931	1.02	1.079	1.575	1.33	0.69	0.70
18	p-xylene	0.332	0.327	0.330	1.02	0.335	0.333	0.33	1.01	0.99
19	4-methyloctane	0.118	0.075	0.097	1.57	0.116	0.106	0.11	1.09	0.87
20	OTHER C9	0.079	0.077	0.078	1.03	0.123	0.078	0.10	1.58	0.78
21	3-methyloctane	0.117	0.111	0.114	1.05	0.114	0.094	0.10	1.21	1.10
22	1,2,3-trimethylcyclohexane	0.225	0.224	0.225	1.01	*0.517*	*0.692*	*0.60*	*0.75*	*0.37*
23	o-xylene	1.632	1.716	1.674	0.95	*3.568*	*5.455*	*4.51*	*0.65*	*0.37*
24	cis, trans-1,2,4-trimethylcycloh	1.281	1.331	**1.306**	0.96	1.217	1.629	**1.42**	0.75	**0.92**
25	1-methyl-2-propylcyclopentane	0.087	0	0.044		0	0	0.00		
26	cis-1-ethyl-3-methylcyclohexan	0.315	0.323	0.319	0.98	0.298	0.365	0.33	0.82	0.96
27	trans-1-ethyl-3-methylcyclohex	0.179	0.174	0.177	1.03	0.148	0.195	0.17	0.76	1.03
28	nonane	0.373	0.374	0.374	1.00	0.376	0.317	0.35	1.19	1.08
29	trans-1-ethyl-2-methylcyclohex	0.139	0.178	0.159	0.78	0.132	0.159	0.15	0.83	1.09
30	cis, trans-1,2,3-trimethylcycloh	0.085	0	0.043		0.08	0.107	0.09	0.75	0.45
31	trans-1-ethyl-4-methylcyclohex	0.348	0.354	0.351	0.98	0.359	0.455	0.41	0.79	0.86
32	cis-1-ethyl-4-methylcyclohexan	0.094	0	0.047		0.086	0.102	0.09	0.84	0.50
33	isopropylbenzene	1.920	1.949	**1.935**	0.99	2.031	2.738	**2.38**	0.74	**0.81**
34	2,3,5-trimethylheptane	0.091	0	0.046		0.064	0	0.03		1.42
35	2,4-dimethyloctane	0.055	0	0.028		0.05	0	0.03		1.10
36	isopropylcyclohexane	0.291	0.234	0.263	1.24	0.196	0.357	0.28	0.55	0.95
37	2,5-dimethyloctane	0.122	0.102	0.112	1.20	0.19	0.085	0.14	2.24	0.81
38	cis-1-ethyl-2-methylcyclohexan	0.137	0.086	0.112	1.59	0.103	0	0.05		2.17
39	propylcyclohexane	0.458	0.386	0.422	1.19	0.39	0.502	0.45	0.78	0.95
40	2,6-dimethyloctane	0.432	0.39	0.411	1.11	0.377	0.245	0.31	1.54	1.32
41	butylcyclopentane	0.125	0	0.063		0.092	0.054	0.07	1.70	0.86
42	1,1,2,3-tetramethylcyclohexane	0.358	0.34	0.349	1.05	0.272	0.217	0.24	1.25	1.43
43	propylbenzene	5.012	5.248	**5.130**	0.96	5.095	6.274	**5.68**	0.81	**0.90**
44	1-ethyl-1,3-dimethylcyclohexa	0.160	0	0.080		0.072	0	0.04		2.22
45	1-ethyl-3-methylbenzene	15.568	16.332	**15.950**	0.95	16.036	16.853	**16.44**	0.95	**0.97**
46	1-ethyl-4-methylbenzene	7.160	7.541	**7.350**	0.95	7.359	7.456	**7.41**	0.99	**0.99**
47	1,3,5-trimethylbenzene	8.413	8.816	**8.615**	0.95	8.502	7.702	**8.10**	1.10	**1.06**
48	2-methylnonane	0.289	0.308	0.299	0.94	0.173	0.162	0.17	1.07	1.78
49	OTHER C10	0.420	0.42	0.420	1.00	0.333	0.329	0.33	1.01	1.27
50	3-ethyloctane	0.248	0.251	0.250	0.99	0.193	0.184	0.19	1.05	1.32
51	1-ethyl-2-methylbenzene	6.206	6.535	**6.370**	0.95	6.222	5.741	**5.98**	1.08	**1.07**
52	3-methylnonane	0.088	0	0.044		0.063	0.076	0.07	0.83	0.63
53	1-methyl-3-isopropylcyclohexa	0.292	0.293	0.293	1.00	0.26	0.193	0.23	1.35	1.29
54	1-methyl-3-isopropylcyclohexa	0.339	0.341	0.340	0.99	0.258	0.225	0.24	1.15	1.41
55	2-ethyl-1,3-dimethylcyclohexa	0.162	0	0.081		0.156	0.118	0.14	1.32	0.59
56	1,2,4-trimethylbenzene	14.656	15.323	**14.990**	0.96	14.735	13.093	**13.91**	1.13	**1.08**
57	1-methyl-2-isopropylcyclohexa	0.361	0.383	0.372	0.94	0.27	0	0.14		2.76
58	diethylcyclohexane	0.410	0	0.205		0.213	0.154	0.18	1.38	1.12
59	decane	1.051	1.106	1.078	0.95	0.968	0.848	0.91	1.14	1.19
60	methyl propylcyclohexane	0.176	0.175	0.176	1.01	0.141	0.148	0.14	0.95	1.21
61	sec-butylbenzene	0.258	0.275	0.267	0.94	0.228	0.224	0.23	1.02	1.18
62	diethylcyclohexane	0.364	0.371	0.368	0.98	0.288	0.247	0.27	1.17	1.37
63	2-ethyl-1,3-dimethylcyclohexa	0.130	0	0.065		0.039	0.045	0.04	0.87	1.55
64	1-methyl-3-isopropylbenzene	0.339	0.435	0.387	0.78	0.326	0.242	0.28	1.35	1.36
65	1,2,3-trimethylbenzene	3.197	3.401	**3.299**	0.94	3.245	2.786	**3.02**	1.16	**1.09**
66	2,5-dimethylnonane	0.239	0	0.120		0	0.085	0.04	0.00	2.81
67	2,6-dimethylnonane	0.411	0.432	0.422	0.95	0.532	0.297	0.41	1.79	1.02

Table 25 - Distribution of Components in Solvent-Based Coating Profiles

	# compounds to weight fraction			
group	***0.50***	***0.75***	***0.90***	***1.00***
2s	10	29	66	167
3s	10	38	99	316
4s	21	51	92	190
5s	24	55	99	203
6s	15	43	80	174
7s	23	50	79	127
8s	18	43	77	155
9s	23	53	89	163
10s	18	39	63	113
11s	16	50	94	204
median	***18***	***47***	***85***	***171***
average	***18***	***45***	***84***	***181***

Table 24 - Composition of Groups by Sample Numbers

Group	sample IDs						
1	Water-based Flats/Low Gloss/Medium Gloss (35)						
	WD01	WD06	WD12	WD23	WD28	WD33	WD48
	WD02	WD07	WD15	WD24	WD29	WD34	WD49
	WD03	WD09	WD16	WD25	WD30	WD35	WD50
	WD04	WD10	WD21	WD26	WD31	WD46	WD51
	WD05	WD11	WD22	WD27	WD32	WD47	WD52
2	Clear Wood Finishes(11)						
	SD27	SD37	WD13	WD18	WD39	WD45	
	SD36	SD38	WD17	WD19	WD40		
3	Solvent-based Industrial Maintenance Coatings (20)						
	SD01	SD04	SD07	SD10	SD13	SD35	SD30
	SD02	SD05	SD31	SD09	SD18	SD25	SD32
	SD03	SD06	SD08	SD12	SD34	SD28	
4	Solvent-based medium gloss/high gloss (7)						
	SD17	SD22	SD24	SD40	SD41	SD42	SD43
5	Solvent-Based Primers and Sealers (5)						
	SD11	SD33	SD45	SD46	SD47		
6	Semi-transparent Stains (7)						
	SD53	SD54	SD55	WD08	WD14	WD20	
7	Traffic Paints (7)						
	SD39	WD37	WD38	WD41	WD42	WD43	WD44
8	Varnishes (4)						
	SD26	SD50	SD51	SD52			
9	Quick-Dry Primers and Non-Flats (3)						
	SD23	SD29	SD44				
10	Graphic Arts Coatings (2)						
	SD48	SD49					
11	Thinning Solvents (5)						
	SD14	SD15	SD16	SD19	SD21		

Figure 12 - Variation Between Calculated and Reported VOC Content for Water-Based Coatings

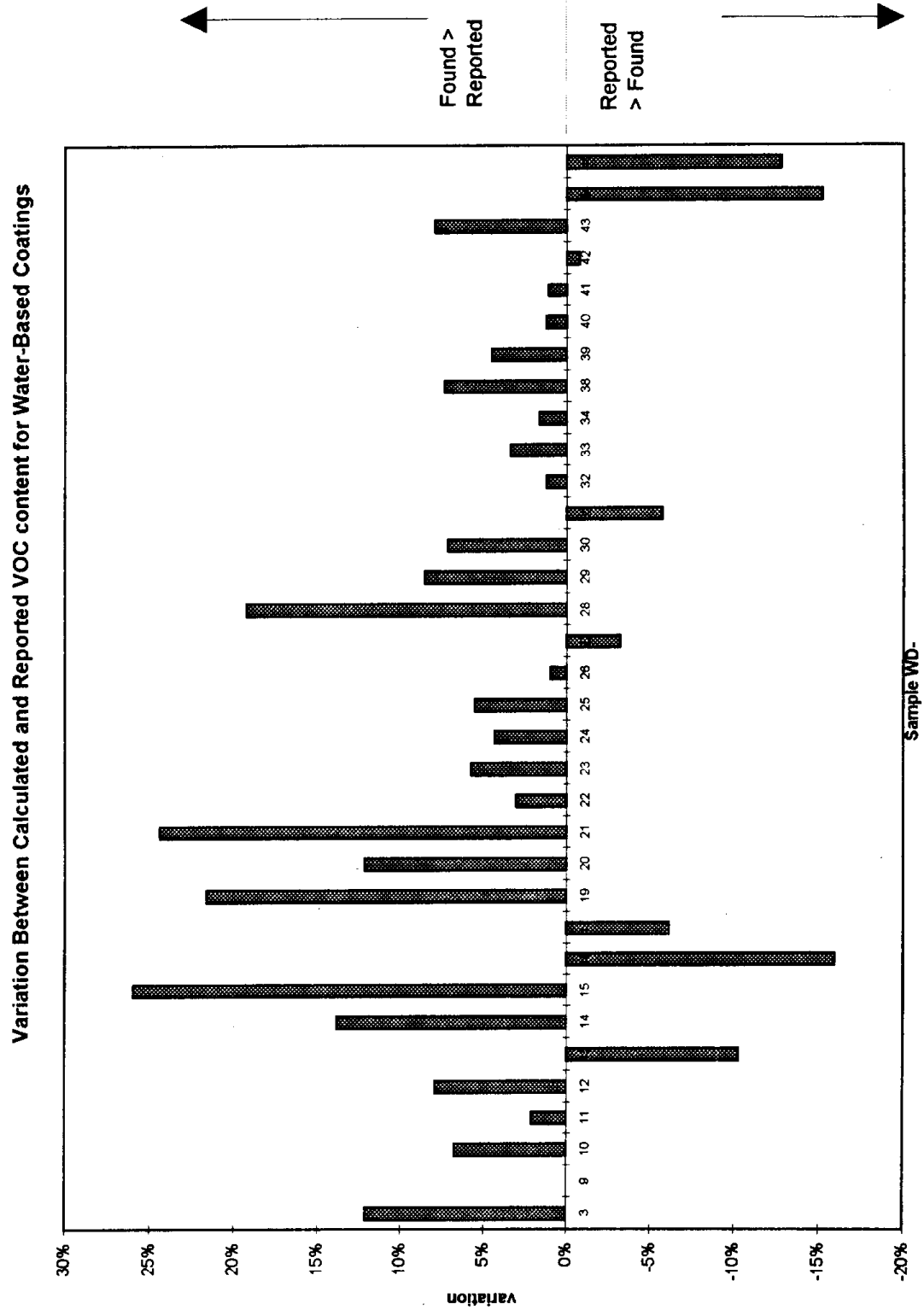


Table 26 - Comparison of Experimental and Reported VOC Values for Water-Based Coatings

	VOC		
sample	**found**	**reported (MSDS)**	**difference**
WD-03	241	215	12%
WD-09	60	60	0%
WD-10	190	178	7%
WD-11	245	240	2%
WD-12	259	240	8%
WD-13	278	310	-10%
WD-14	206	181	14%
WD-15	170	135	26%
WD-16	168	200	-16%
WD-17	349	372	-6%
WD-19	276	227	22%
WD-20	369	329	12%
WD-21	199	160	24%
WD-22	170	165	3%
WD-23	258	244	6%
WD-24	218	209	4%
WD-25	134	127	6%
WD-26	106	105	1%
WD-27	179	185	-3%
WD-28	124	104	19%
WD-29	153	141	9%
WD-30	124	116	7%
WD-31	84	89	-6%
WD-32	122	121	1%
WD-33	249	241	3%
WD-34	223	219	2%
WD-38	59	55	7%
WD-39	241	231	4%
WD-40	234	231	1%
WD-41	141	139	1%
WD-42	69	70	-1%
WD-43	119	110	8%
WD-44	156	184	-15%
WD-46	218	250	-13%

Average	**4%**

V. Summary and Conclusions

In this study, the nature of emissions from architectural and industrial maintenance coatings was examined. Coating materials for investigation were arranged into 11 main groups, based on similarity of use, emissions, and sales-weighted VOC values. Three of these groups contained both water - and solvent -based coatings. Accordingly, each of these three categories (Group 2, 6, and 7) were sub-divided into water and solvent sub-categories (2w, 2s, 6w, 6s, 7w,7s), producing a total of 14 Groups. For consistency, a one letter suffix (either w or s) was appended to the group numbers, to indicate the nature of the carrier system (water- or solvent-based). Table 28 summarizes these groups. A number of approaches were used to determine the emission species profile for 106 coating samples.

An emission chamber was constructed, based on a disposable 1 quart friction-topped steel paint can. The sampling container was placed in a forced draft convection oven, and heated to 110°C for 1 hour, consistent with ASTM Method 2369. Emissions from coating samples were swept through a manifold containing three sorbent tubes by a stream of ultra-pure nitrogen, with the flow through each tube regulated by a separate mass flow controller. Two styles of sorbent tubes were evaluated: stainless steel and glass, filled with a multisorbent. The steel tubes were analyzed by thermal desorption, the glass tubes by solvent extraction. The chamber was validated using a series of characterized coating samples. The polar solvents found in water-based coating samples did not lend themselves well to efficient thermal desoprtion and transfer to the inlet system of the gas chromatograph used for the study. The solvent extraction of glass sorbent tubes produced emission profiles that were consistent with the composition of known samples. When applied to a variety of coatings, the chamber method revealed a tendency for high boiling solvents to remain associated with the paint film, even after 1 hour of drying at 110°C. This was verified by direct analysis of the dried paint film.

A number of solvent-based coating samples were evaluated by the chamber method. Initial tests using the thermal desorption of the steel sorbent tubes showed that the VOC loading on these tubes was too high, producing an overload on the chromatographic column, with the resulting loss of column efficiency and resolution. A dilution system was fabricated, to allow the effluent from the thermal desorption unit to be split prior to the chromatographic inlet. While this improved the chromatography, resolution was still not sufficient for the complete analysis of solvent coatings with complex solvent systems.

Direct methods of analysis were developed to address the limitations of the emission chamber. For water-based coatings, a direct method, involving dilution with solvent, centrifugation, and gas chromatography of the centrifugate proved successful. Detailed emission profiles were obtained for 52 water-based coatings.

A similar method was tested for the direct analysis of solvent-based coatings. This approach worked well for coatings with simple solvent systems. Detailed emission profiles were obtained for 10 solvent-based coatings, using this method. A large number of solvent-based coating samples employ mineral spirits as a major solvent. This is actually a complex mixture of hydrocarbons. Identifying a solvent that could extract these materials from a paint, and not interfere with the subsequent analysis proved to be impossible. A method based on the removal of solvents from the coating sample by distillation was developed. The coating sample was dispersed in a mixture of (essentially) non-volatile dioctyl phthalate and high boiling tetradecane. The mixture was distilled under reduced pressure, until the tetradecane distilled over. The distillate, collected in a liquid nitrogen cooled receptacle, contained all of the solvent components of the original coating samples, but none of the pigment or polymer. Direct injection of the distillate into a gas chromatograph produced good detection of even minor components. Using this approach, detailed emission profiles were obtained for 54 solvent-based coating samples. These species profiles were obtained using a combination of GC-FID and GC-MS for each sample.

Table 27 - Comparison of Identified and Reported Species in Solvent-Based Coatings

Sample	Found by GC analysis but not on MSDS
SD03	methanol, ethylene glycol, 2-heptanone, neopentyl glycol
SD04	methanol, ethylene glycol, 2-heptanone, neopentyl glycol, xylenes
SD06	methanol, 1-butanol, butyl acetate, 2-heptanone, 2,2,4-trimethyl-1,3-pentanediol
SD15	ethanol
SD29	methyl ethyl ketone, propanol, butyl acetate
SD31	isobutyl alcohol, acetophenone
SD35	butyl acetate
SD37	ethanol

Table 28 - Summary of Coating Groups

group #	working group name
1w	water-based flats/low gloss/medium gloss
2w	water-based clear wood finishes(clear sanding sealers, watersealers, lacquers)
2s	solvent based clear wood finishes(clear sanding sealers, watersealers, lacquers)
3s	industrial maintenance coatings
4s	solvent based medium gloss/high gloss
5s	solvent based primers and sealers
6w	water-based semitransparent stains
6s	solvent based semitransparent stains
7w	water-based traffic paints
7s	solvent based traffic paints
8s	solvent based varnishes
9s	solvent based quick dry primers and enamels
10s	solvent based graphic arts coatings
11s	thinning solvent

Identification of the solvent components was made by the comparison of experiment retention indices with a library of such indices developed in our laboratory. Peak assignments were verified by examination of the mass spectra against a NIST database.

These individual profiles were arranged into composite group profiles.

The procedures described in this report produced detailed species profiles, with as many as several hundred components being identified. The overall identification rate of VOC species was high. For water based samples, 100% of the VOC mass was identified in all but four samples. In these cases, a few percent of unknown species were detected. For the solvent-based coatings, the identification rate was not quite this good, but even in the worst case, over 90% of the VOC mass was identified. For those components not positively identified, a carbon number was assigned, based on the retention index of the peak.

Appendix A

STANDARD OPERATING PROCEDURES FOR SAMPLING VOC EMISSIONS

5. PROCEDURE

5.1 Establish flow rates

5.1.1 Set up mass flow controllers for desired flow rates.
5.1.2 Check total flow rate from nitrogen tank. Adjust this, using a soap bubble flowmeter to within 10 % of 1000 mL/minute.

5.2 Leak Check Sampling Chamber

5.2.1 Place four 10 mm glass balls and six 5 mm glass balls into the cleaned sampling chamber.
5.2.2 Place a Teflon sheet gasket on the sealing surface of a pre-cleaned sampling chamber (1 quart paint can).
5.2.3 Attach the top of the can, and tap uniformly to seat the friction lid.
5.2.4 Attach a nitrogen line to the inlet port of the chamber.
5.2.5 Attach a tee to the outlet port of the can. Leave one arm of the tee open to the atmosphere. Attach a Magnehelic gauge (0-5" water) to the other arm of the tee.
5.2.6 Enable the flow of nitrogen into the sampling chamber, and purge the chamber for 5 minutes.
5.2.7 At the end of the purge period. close the outlet valve, and allow the nitrogen to pressurize the can to 5" of water. Close the inlet valve and monitor the pressure for 1 minute. A drop of 1" of water corresponds to a leak rate of 2.4 mL/minute. If the pressure drops more than 1" of water in 1 minute, re-seal the can, and repeat the leak check. Isolate and eliminate any leaks in the system, until the system passes the leak test.
5.2.8 Remove nitrogen lines from sampling chamber.

5.3 Sampling

5.3.1 Before use, rinse the sampling chamber with methanol, and dry in an oven at 110°C.
5.3.2 Remove the protective end caps from one of the sorbent cartridges, and install the cartridge into the sampling train. Repeat for the remaining sorbent cartridges.
5.3.2 Agitate the sealed vial containing the coating sample thoroughly, using a mechanical shaker or vortex mixer. Attach a stub of Teflon tubing to a disposable 5 mL syringe, and draw a sample of coating from the middle of the agitated sample vial.
5.3.3 Replace the Teflon tubing with a stainless steel needle, and use a balance to determine the mass of the syringe/needle coating sample.
5.3.4 Inject the appropriate amount of sample, corresponding to about 0.5 grams of coating, through the septum into the sealed and leak-checked sampling chamber.
5.3.5 Re-weigh the syringe/needle combination to determine the mass of coating delivered into the sampling chamber.
5.3.6 Swirl the sampling chamber for one minute, allowing the mixing balls to spread out the coating.

STANDARD OPERATING PROCEDURE

FOR SAMPLING VOC EMISSIONS USING A SMALL CHAMBER

1. SCOPE

1.1 This method can be used to sample VOCs emitted from water- and solvent-borne paint and coating samples.
1.2 The ultimate use of the method involves the determination of VOC species profiles for paint and coating samples.

2. METHOD SUMMARY

2.1 A known mass of the coating material is sealed into a small chamber.
2.2 The sealed chamber is placed into a forced convection oven maintained at 110°C for 1 hour.
2.3 The VOCs emitted during the drying period are swept out of the chamber, using a stream of high purity nitrogen.
2.4 The nitrogen stream is led into a manifold, and metered by mass flow controllers into three separate sorbent tubes containing multisorbent.
2.5 Once sampled, the sorbent tubes are analyzed according to EPA Method TO2, using thermal desorption followed by separation on a fused silica capillary GC column.

3.0 EQUIPMENT

3.1. Custom small chamber, equipped with a friction top with quick connect fittings, and a septum adapter
3.2. Sorbent tubes containing multisorbent (Supelco Carbotrap 300)
3.3. Mass flow controllers, capable of controlling flow rates in the range of 10 to 100 mL/minute

4. SUB-SAMPLING

4.1 Consistent with ASTM procedure D 3925 (Standard Practice for Sampling Liquid Paints and Related Coatings), agitate the coating samples in the original containers on a mechanical shaker until homogenized.
4.2 Open the original container, and fill the appropriate number of pre-cleaned, 40 mL glass vials. For normal samples, five 40 mL vials will be filled. For validation samples, ten 40 mL samples will be obtained. Be sure all caps are tightly secured on the vials.

Chamber Sampling Check List

Preparation

☐ Rinse can with methanol, followed by water; dry in oven
☐ Rinse glass beads with methanol, followed by water; dry in oven
☐ Check tightness of all Teflon fittings
☐ Set up flow from N_2 tank to 82 ball units (center)
☐ Set mass flow controllers to desired values
☐ Install new septum
☐ Load glass beads into chamber
☐ Install 2 layers of Teflon tape onto can bottom
☐ Attach can lid; seal with finger pressure; open can tee valve

Leak Check

☐ Attach N_2 inlet from can to oven; Allow N_2 to flow for 5 minutes
☐ Shut off flow; Close tee valve; Attach Magnehelic to valve on can tee
☐ Open N_2, allowing system pressure to build to 2" H_2O, then disconnect N_2 line
☐ Monitor pressure at end of 60 seconds; if less than 1", reseal can, and repeat leak test
☐ Remove Magnehelic gauge; Shut off can tee valve

Sampling

☐ Install sorbent tubes, bottom ends first; Replace insulation around base of tubes
☐ Install MFC manifold to upper end of sorbent tubes
☐ Check power and setpoints of MFC's
☐ Verify flow of N_2 set at 82 ball units; turn N_2 valve to <OFF>
☐ Fill syringe with sample; weigh
☐ Be sure can tee valve is closed; Dispense into can; re-weigh
☐ Close vacuum shutoff valve
☐ Put can in oven, attach inlet and outlet lines
☐ Turn on vacuum pump; open vacuum valve
☐ Open all MFC valves; Move N_2 valve to <ON>; QUICKLY Open can tee valve
☐ Turn on oven; Install air cooling manifold
☐ Turn on cooling air flow
☐ Monitor sorbent tube temperatures

Final Steps

☐ Close MFC valves
☐ Close vacuum shutoff valve; shut off vacuum pump
☐ Shut off N_2 flow; close main cylinder valve
☐ Double check sampling and tube information
☐ Remove MFC manifold from upper end of sorbent tubes; Cap each open tube
☐ Remove bottom ends of sorbent tubes; Cap the open ends
☐ Disconnect quick connects when cool

5.3.7 Place the chamber into a forced draft oven maintained at 100°C.
5.3.8 With the nitrogen purge gas valve in the OFF position, push the can up to engage the inlet and outlet quick connects mounted in the oven.
5.3.9 Start the sampling timer
5.3.10 Open the isolation valve leading to the sorbent tubes, and open the nitrogen purge valve.
5.3.11 Collect the emissions from the sampling chamber for a period of one hour.
5.3.12 At the end of the sampling period, close the nitrogen purge valve, and close the isolation valves on both sides of the sorbent tubes.
5.3.13 Remove the first sorbent tube, replacing the end caps securely. Repeat this for the remaining sorbent tubes.
5.3.14 Transport the used sorbent cartridges to the analytical laboratory for analysis.

5. PROCEDURE

5.1 Sampling for Water-Based Coatings (Direct Method)

5.1.1 Agitate the sealed vial containing the coating sample thoroughly, using a mechanical shaker or vortex mixer.
5.1.2 Dispense 10.00 mL of solvent into a clean vial. Use methanol as the solvent, with 2-ethyl hexanol as internal standard. If methanol is present in the formulation, use DMF as solvent, with n-propanol as internal standard.
5.1.3 Seal the vial with a septum cap.
5.1.4 Attach a stub of Teflon tubing to a disposable 5 mL syringe, and draw a sample of coating from the middle of the agitated sample vial.
5.1.5 Replace the Teflon tubing with a stainless steel needle, and use a balance to determine the mass of the syringe/needle coating sample.
5.1.6 Inject the appropriate amount of sample, corresponding to about 0.5 grams of coating, through the septum into the sealed vial.
5.1.7 Re-weigh the syringe/needle combination to determine the mass of coating delivered into the vial.
5.1.8 Mix the vial thoroughly, then centrifuge for 5 minutes at 100 RPM, to facilitate settling.
5.1.9 Remove a 1.00 mL aliquot of centrifugate from the vial, and dilute it to 25.00 mL with solvent. Seal the diluted solution in a septum capped vial.
5.1.10 For analysis, inject a 1 μL aliquot of the diluted sample into a GC for quantitation.
5.1.11 Perform additional dilution(s) if instrumental response is not in the linear region.

5.2 Sampling for Solvent-Based Coatings (Direct Method - Solvent Dilution)

5.2.1 Agitate the sealed vial containing the coating sample thoroughly, using a mechanical shaker or vortex mixer
5.2.2 Dispense 10.00 mL of solvent into a clean vial. Use methyl t-butyl ether as the solvent. Add 1.00 mL of diphenyl methane as internal standard.
5.2.3 Seal the vial with a septum cap
5.2.4 Attach a stub of Teflon tubing to a disposable 5 mL syringe, and draw a sample of coating from the middle of the agitated sample vial.
5.2.5 Replace the Teflon tubing with a stainless steel needle, and use a balance to determine the mass of the syringe/needle/ coating sample.
5.2.6 Inject the appropriate amount of sample, corresponding to about 0.5 grams of coating, through the septum into the sealed vial.
5.2.7 Re-weigh the syringe/needle combination to determine the mass of coating delivered into the vial.
5.2.8 Mix the vial thoroughly, then centrifuge for 5 minutes at 100 RPM, to facilitate settling.

STANDARD OPERATING PROCEDURE

FOR SAMPLING VOC EMISSIONS

FROM BULK COATING MATERIALS

1. SCOPE

1.1 This method can be used to sample VOCs emitted from water- and solvent-borne paint and coating samples

1.2 The ultimate use of the method involves the determination of VOC species profiles for paint and coating samples.

2. METHOD SUMMARY

2.1 A clean vial is filled with a known volume of diluent, and a known amount of an internal standard solution. The vial is sealed with a septum cap.

2.2 A known mass of the coating material is injected into the vial through the septum top.

2.3 The sample is mixed by shaking, and centrifuged to separate the solids.

2.4 The centrifugate is diluted with solvent to a concentration that falls within the linear range of the analytical technique.

2.5 Alternatively, the solvents may be removed from the coating sample by distillation.

2.5 An aliquot of the diluted sample is injected directly into a GC inlet, for separation on a fused silica capillary GC column.

3. EQUIPMENT

3.1. Septum capped vials

3.2. Disposable syringe for dispensing coating samples

4. SUB-SAMPLING

4.1 Consistent with ASTM procedure D 3925 (Standard Practice for Sampling Liquid Paints and Related Coatings), agitate the coating samples in the original containers on a mechanical shaker until homogenized.

4.2 Open the original container, and fill the appropriate number of pre-cleaned, 40 mL glass vials. For normal samples, five 40 mL vials will be filled. For validation samples, ten 40 mL samples will be obtained. Be sure all caps are tightly secured on the vials.

Appendix B

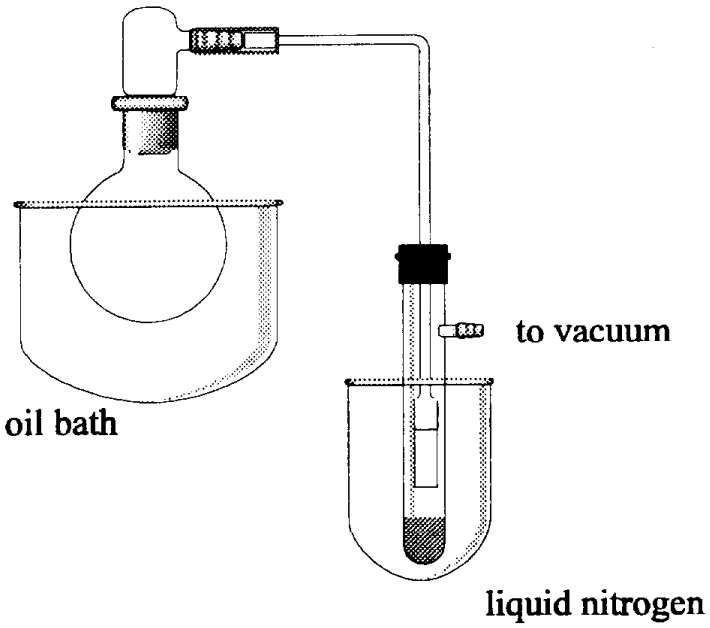
COMPARISON OF SPECIES ANALYSIS WITH MSDS

5.2.9 Remove a 1.00 mL aliquot of centrifugate from the vial, and dilute it to 25.00 mL with solvent. Seal the diluted solution in a septum capped vial.
5.2.10 For analysis, inject a 1 μL aliquot of the diluted sample into a GC for quantitation.
5.2.11 Perform additional dilution(s) if instrumental response is not in the linear region.

5.3 Sampling for Solvent-Based Coatings (Direct Method - Distillation)

5.3.1 Agitate the sealed vial containing the coating sample thoroughly, using a mechanical shaker or vortex mixer
5.3.2 Dispense between 1.0000 and 3.0000 grams of the coating material into a 100 mL round-bottom flask containing 5.0 grams of dioctylphthalate and 1.5 gram of tetradecane.
5.3.3 Assemble the glassware as shown in Figure 1.

Figure 1 - Distillation Apparatus



5.3.4. Fill the condensing Dewar with liquid nitrogen.
5.3.5 Attach the vacuum pump, and establish a vacuum between 0.3 and 0.5 torr
5.3.6 Gradually increase the temperature of the mixture, until it reaches 120°C. Maintain this temperature for 5 to 10 minutes, until all solvents have been distilled.
5.3.7 At the end of the distillation, remove the receiving tube from the liquid nitrogen bath, and allow its contents to melt.
5.3.8 Centrifuge the tube , and transfer the homogenized contents to a screw-capped vial.
5.3.9 Analyze by GC, as in 5.2.10.

WD-11	Found	Reported in MSDS
% PG	4.02	<5.0
% DB	0.66	None
% TX	4.58	None
% DPE		<5.0
%Total VOC	9.26	
VOC, Found	245	
VOC, Reported	240	

WD-12	Found	Reported in MSDS
% PG	2.96	<5.0
%PnB	0.74	None
%DPM	0.66	None
% DB	1.42	None
% TX	4.06	None
%Total VOC	9.83	
VOC, Found	259	
VOC, Reported	240	

WD-13	Found	Reported in MSDS
% PG	2.06	<5.0
% EB	0.44	None
%PnB	1.20	<5.0
%DPM	3.75	<5.0
%NMP	1.47	<5.0
% TX	2.46	
%Total VOC	11.38	
VOC, Found	278	
VOC, Reported	310	

WD-14	Found	Reported in MSDS
% PG	2.54	<5.0
% DB	0.87	1
%Total VOC	3.40	
VOC, Found	206	
VOC, Reported	181	

WD-15	Found	Reported in MSDS
% PG	4.07	3
% TX	1.94	2
% Formaldehyde	0.007	0.003
%Total VOC	6.02	
VOC, Found	170	
VOC, Reported	135	

WD-16	Found	Reported in MSDS
% PG	5.08	None
% TX	0.95	None
%Total VOC	6.02	
VOC, Found	168	
VOC, Reported	200	

WD-03	Found	Reported in MSDS
% PG		
% DB	0.34	None
% TX	3.21	None
%UK	0.22	
%Total VOC	9.24	
VOC, Found	241	
VOC, Reported	215	

WD-04	Found	Reported in MSDS
% PG	3.06	None
% HG	1.40	1 to 2
% DB	0.44	None
% TX	0.92	1
%Total VOC	5.82	

WD-05	Found	Reported in MSDS
% EG	0	5
% PG	3.62	None
% TX	0.92	5
%Total VOC	4.54	

WD-06	Found	Reported in MSDS
% PG	7.26	None
% OMS	0.54	None
% TX	0.74	None
%Total VOC	8.54	

WD-08	Found	Reported in MSDS
%IPA	0.63	None
% PG	0.90	None
%PnP	0.90	None
% EB	1.09	1
%DPnB	0.93	None
%UK	0.15	None
%Total VOC	4.60	

WD-09	Found	Reported in MSDS
% EG	0.65	0.75
% TX	0.98	None
% Formaldehyde	0.001	0.003
% Acetaldehyde	0.013	None
%Total VOC	1.63	
VOC, Found	60	
VOC, Reported	60	

WD-10	Found	Reported in MSDS
% EG	2.18	2.47
% TX	3.89	3
%Total VOC	6.07	
VOC, Found	190	
VOC, Reported	178	

WD-24	Found	Reported in MSDS
% EG	4.91	5
% TX	2.12	<5.0
%Total VOC	7.03	
VOC, Found	218	
VOC, Reported	209	

WD-25	Found	Reported in MSDS
% EG	2.06	2
% TX	1.79	<5.0
%Total VOC	3.85	
VOC, Found	134	
VOC, Reported	127	

WD-26	Found	Reported in MSDS
% EG	1.77	2
% PG	0.33	None
% TX	1.66	<5.0
%Total VOC	3.76	
VOC, Found	106	
VOC, Reported	105	

WD-27	Found	Reported in MSDS
% PG	0.35	None
%DM	5.52	5
% DB	0.67	None
%Total VOC	6.54	
VOC, Found	179	
VOC, Reported	185	

WD-28	Found	Reported in MSDS
% PG	1.88	<5.0
% TX	1.11	<5.0
%Total VOC	2.99	
VOC, Found	124	
VOC, Reported	104	

WD-29	Found	Reported in MSDS
% PG	3.22	<5.0
% TX	2.08	<5.0
%Total VOC	5.30	
VOC, Found	153	
VOC, Reported	141	

WD-30	Found	Reported in MSDS
% PG	2.50	<5.0
% DB	0.14	None
% TX	1.34	<5.0
%Total VOC	3.99	
VOC, Found	124	
VOC, Reported	116	

WD-31	Found	Reported in MSDS
% EG	1.18	1
% TX	1.60	0
%UK	0.04	
%Total VOC	2.78	
VOC, Found	84	
VOC, Reported	89	

WD-17	Found	Reported in MSDS
propylene glycol	4.46	None
p-xylene	0.04	None
o-xylene	0.13	None
cumene	0.06	None
propylbenzene	0.17	None
benzene, 1-ethyl-3-methyl	0.67	None
benzene, 1-ethyl-4-methyl	0.29	None
benzene, 1,3,5-trimethyl	0.37	None
benzene, 1-ethyl-2-methyl	0.23	None
benzene, 1,2,4-trimethyl	1.14	None
benzene, 1,2,3-trimethyl	0.19	None
PM	4.12	None
DPM	2.20	None
%Total VOC	14.08	
Total Rptd	14.66	
VOC, Found	349	
VOC, Reported	372	

WD-19	Found	Reported in MSDS
% PG	2.28	Listed
%TEA	1.00	None
%DPM	3.88	None
%NMP	7.20	5
%Total VOC	14.36	
VOC, Found	276	
VOC, Reported	227	

WD-20	Found	Reported in MSDS
%IPA	0.32	None
% PG	7.08	5
% EB	0.19	None
%DE	0.44	None
%NMP	0.24	None
%Total VOC	8.28	
VOC, Found	369	
VOC, Reported	329	

WD-21	Found	Reported in MSDS
% PG	3.99	5
% TX	1.77	None
%Total VOC	5.77	
VOC, Found	199	
VOC, Reported	160	

WD-22	Found	Reported in MSDS
% PG	3.81	5
% TX	1.71	None
%Total VOC	5.52	
VOC, Found	170	
VOC, Reported	165	

WD-23	Found	Reported in MSDS
% PG	6.08	5
% DB	0.38	None
% TX	2.90	None
%Total VOC	9.36	
VOC, Found	258	
VOC, Reported	244	

WD-43	Found	Reported in MSDS
%MeOH	3.31	2 to 3
% DB	1.83	1 to 2
%Total VOC	5.14	
VOC, Found	119	
VOC, Reported	110	

WD-44	Found	Reported in MSDS
%MeOH	3.93	Listed
%EtOH	0.86	5
% PG	0.71	5
% DB	0.92	None
% TX	0.60	None
%Total VOC	7.03	
VOC, Found	156	
VOC, Reported	184	

WD-46	Found	Reported in MSDS
%IPA	0.47	<5.0
%2BuOH	2.16	3
% EB	3.45	3
% DB	0.64	<5.0
%Total VOC	6.72	
VOC, Found	218	
VOC, Reported	250	

WD-32	Found	Reported in MSDS
% EG	1.58	2
% DB	0.13	None
% TX	1.28	0
%UK	0.10	
%Total VOC	2.99	
VOC, Found	122	
VOC, Reported	121	

WD-33	Found	Reported in MSDS
% EG	3.36	4
%DM	0.90	1
% DB	0.34	None
% TX	4.02	0
%Total VOC	9.00	
VOC, Found	249	
VOC, Reported	241	

WD-34	Found	Reported in MSDS
% EG	0	5
% PG	5.11	None
% TX	1.95	5
%Total VOC	7.07	
VOC, Found	223	
VOC, Reported	219	

WD-38	Found	Reported in MSDS
%MeOH	0.84	None
% DB	1.15	None
%Total VOC	1.98	
VOC, Found	59	
VOC, Reported	55	

WD-39	Found	Reported in MSDS
% EB	9.44	9
%DBP	0.92	2
%Total VOC	10.36	
VOC, Found	241	
VOC, Reported	231	

WD-40	Found	Reported in MSDS
% EB	9.19	10
%DBP	0.77	2
%Total VOC	9.95	
VOC, Found	234	
VOC, Reported	231	

WD-41	Found	Reported in MSDS
% EG	2.93	2.99
% PG	0.16	None
% DB	0.17	None
% TX	1.78	2
%Total VOC	5.04	
VOC, Found	141	
VOC, Reported	139	

WD-42	Found	Reported in MSDS
%MeOH	0.15	None
%EtOH	1.16	None
%IPA	0.11	None
% EB	0.09	None
% DB	0.68	None
%Total VOC	2.19	
VOC, Found	69	
VOC, Reported	70	

Appendix C

SPECIES PROFILES FOR WATER-BASED COATINGS

Water-Based Coatings	WD14	WD15	WD16	WD17	WD18	WD19	WD20	WD21	WD22	WD23	WD24	WD25	WD26
sec-butyl alcohol													
1-amino-2-methyl-2-propanol													
diethylene glycol butyl ether	0.2543									0.0411			
dibutyl phthalate													
diethylene glycol ethyl ether							0.0535						
diethylene glycol													
diethylene glycol methyl ether													
dipropylene glycol methyl ether					0.1121								
dipropylene glycol butyl ether													
2-butoxyethanol							0.0228						
ethylene glycol											0.6989	0.5346	0.4697
ethanol													
hexylene glycol													
isopropyl alcohol							0.0388						
methyl amyl ketone					0.1153								
methanol													
N-methylpyrrolidone					0.7727	0.7760	0.0320						
propylene glycol	0.7457	0.6732	0.8576			0.2240	0.8528	0.6926	0.6903	0.6493			0.0885
2-methoxy-1-propanol				1.0000									
1-butoxy-2-propanol													
1-propoxy-2-propanol													
glycerin													
Texanol		0.3268	0.1424					0.3074	0.3097	0.3096	0.3011	0.4654	0.4419
unknown C8													
unknown C9													
unknown C12													
TOTAL													
	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

Water-Based Coatings	WD1	WD2	WD3	WD4	WD5	WD6	WD7	WD8	WD9	WD10	WD11	WD12	WD13
sec-butyl alcohol													
1-amino-2-methyl-2-propanol													
diethylene glycol butyl ether		0.0567	0.0355	0.0735			1.0000				0.0690	0.1439	
dibutyl phthalate													
diethylene glycol ethyl ether													
diethylene glycol													
diethylene glycol methyl ether													
dipropylene glycol methyl ether												0.0672	0.3044
dipropylene glycol butyl ether								0.2029					
2-butoxyethanol								0.2377					0.0353
ethylene glycol		0.4515				0.0265			0.3989	0.3594			
ethanol													
hexylene glycol				0.2440									
isopropyl alcohol								0.1367					
methyl amyl ketone													
methanol													
N-methylpyrrolidone													0.1459
propylene glycol	0.7692	0.1004	0.5993	0.5266	0.7973	0.8205		0.1950			0.4457	0.3007	0.1892
2-methoxy-1-propanol													
1-butoxy-2-propanol												0.0749	0.0956
1-propoxy-2-propanol								0.1949					
glycerin													
Texanol	0.2308	0.3914	0.3419	0.1560	0.2027	0.0864			0.6011	0.6406	0.4852	0.4133	0.2297
unknown C8													
unknown C9						0.0666							
unknown C12			0.0232					0.0328					
TOTAL	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

Water-Based Coatings	WD40	WD41	WD42	WD43	WD44	WD45	WD46	WD47	WD48	WD49	WD50	WD51	WD52
sec-butyl alcohol						0.0500	0.3250						
1-amino-2-methyl-2-propanol								0.1094					0.0277
diethylene glycol butyl ether		0.0335	0.3081	0.3662	0.1253		0.0921		0.1371	0.0828	0.0358	0.0985	
dibutyl phthalate	0.0741												
diethylene glycol ethyl ether													
diethylene glycol													0.3422
diethylene glycol methyl ether													
dipropylene glycol methyl ether													
dipropylene glycol butyl ether													
2-butoxyethanol	0.9259		0.0435				0.5105						
ethylene glycol		0.5812								0.7082		0.6190	
ethanol			0.5297		0.1230								
hexylene glycol													
isopropyl alcohol			0.0509			0.9500	0.0724						
methyl amyl ketone													
methanol			0.0678	0.6338	0.5635								
N-methylpyrrolidone													
propylene glycol		0.0311			0.0991				0.2949		0.6351		0.0461
2-methoxy-1-propanol													
1-butoxy-2-propanol													
1-propoxy-2-propanol													
glycerin													
Texanol		0.3541			0.0891			0.8906	0.5679	0.1789	0.3292	0.2825	0.5408
unknown C8													0.0433
unknown C9													
unknown C12										0.0301			
TOTAL													
	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

Water-Based Coatings	average	zero values	present in samples
sec-butyl alcohol	0.0072	50	2
1-amino-2-methyl-2-propanol	0.0026	50	2
diethylene glycol butyl ether	0.0725	29	23
dibutyl phthalate	0.0031	50	2
diethylene glycol ethyl ether	0.0010	51	1
diethylene glycol	0.0066	51	1
diethylene glycol methyl ether	0.0182	50	2
dipropylene glycol methyl ether	0.0093	49	3
dipropylene glycol butyl ether	0.0039	51	1
2-butoxyethanol	0.0517	45	7
ethylene glycol	0.1271	38	14
ethanol	0.0126	50	2
hexylene glycol	0.0047	51	1
isopropyl alcohol	0.0240	47	5
methyl amyl ketone	0.0022	51	1
methanol	0.0429	47	5
N-methylpyrrolidone	0.0332	48	4
propylene glycol	0.2716	21	31
2-methoxy-1-propanol	0.0192	51	1
1-butoxy-2-propanol	0.0033	50	2
1-propoxy-2-propanol	0.0037	51	1
glycerin	0.0162	51	1
Texanol	0.2593	15	37
unknown C8	0.0008	51	1
unknown C9	0.0013	51	1
unknown C12	0.0017	49	2
TOTAL			

Appendix D

SPECIES PROFILES FOR SOLVENT-BASED COATINGS

SD01	
Compound	fraction
2-Pentanone	0.0825
Butyl Acetate	0.3275
Ethylbenzene	0.0130
m-Xylene	0.0397
p-Xylene	0.0132
2-Heptanone	0.4992
o-Xylene	0.0248
Total	1.0000

SD02	
Compound	fraction
2-Butanone	0.0523
Butyl Acetate	0.4022
Ethylbenzene	0.0039
m-Xylene	0.0097
p-Xylene	0.0032
2-Heptanone	0.5243
o-Xylene	0.0044
Total	1.0000

SD03	
Compound	fraction
Methanol	0.0592
1-Butanol	0.0572
Ethylene glycol	0.0452
1-Methoxy-2-acetoxypropane	0.0000
2-Heptanone	0.0974
Neopentyl Glycol	0.0118
Butyl Cellosolve	0.3638
Ethyl-3-ethoxypropionate	0.1409
Texanol	0.2069
Ethylbenzene	0.0024
m-Xylene	0.0069
p-Xylene	0.0025
o-Xylene	0.0058
Total	1.0000

SD04	
Compound	fraction
Methanol	0.1900
1-Butanol	0.3256
Ethylene glycol	0.0575
1-Methoxy-2-acetoxypropane	0.0000
2-Heptanone	0.1662
Neopentyl Glycol	0.0156
Butyl Cellosolve	0.0715
Ethyl-3-ethoxypropionate	0.0607
Texanol	0.0565
Ethylbenzene	0.0045
m-Xylene	0.0131
p-Xylene	0.0047
o-Xylene	0.0136
Isopropylbenzene	0.0004
n-propylbenzene	0.0008
1-Methyl-3-ethylbenzene	0.0037
1-Methyl-4-ethylbenzene	0.0016
1,3,5-Trimethylbenzene	0.0023
1-Methyl-2-ethylbenzene	0.0013
1,2,4-Trimethylbenzene	0.0079
i-Butylbenzene	0.0000
1-Methyl-3-isopropylbenzene	0.0001
1,2,3-Trimethylbenzene	0.0015
Indan	0.0002
1,3-Diethylbenzene	0.0001
1-Methyl-3-propylbenzene	0.0001
1-Methyl-4-propylbenzene	0.0003
1-Methyl-2-propylbenzene	0.0000
1,4-Dimethyl-2-ethylbenzene	0.0001
1,4-Dimethyl-2-ethylbenzene	0.0001
1,2-Dimethyl-4-ethylbenzene	0.0002
1-Ethyl-4-isopropylbenzene	0.0001
1,2,4,5-tetramethylbenzene	0.0001
Total	1.0000

SD05	
Compound	fraction
1-Butanol	0.1029
Butyl Acetate	0.0190
1-Methoxy-2-acetoxypropane	0.1211
Butyl Cellosolve	0.0874
Isophorone	0.1058
o-Xylene	0.0606
Isopropylbenzene	0.0088
n-propylbenzene	0.0189
1-Methyl-3-ethylbenzene	0.0886
1-Methyl-4-ethylbenzene	0.0399
1,3,5-Trimethylbenzene	0.0562
1-Methyl-2-ethylbenzene	0.0311
1,2,4-Trimethylbenzene	0.1906
s-Butylbenzene	0.0006
i-Butylbenzene	0.0007
1-Methyl-3-isopropylbenzene	0.0020
1,2,3-Trimethylbenzene	0.0354
Indan	0.0043
1,3-Diethylbenzene	0.0013
1-Methyl-3-propylbenzene	0.0033
1-Methyl-4-propylbenzene	0.0063
1-Methyl-2-propylbenzene	0.0009
1,4-Dimethyl-2-ethylbenzene	0.0022
1,4-Dimethyl-2-ethylbenzene	0.0019
1,2-Dimethyl-4-ethylbenzene	0.0037
1,3-Dimethyl-2-ethylbenzene	0.0002
2-Phenyl-2-methylbutane	0.0002
1,2-Dimethyl-3-ethylbenzene	0.0002
1-Ethyl-2-isopropylbenzene	0.0005
1-Ethyl-4-isopropylbenzene	0.0017
1,2,4,5-tetramethylbenzene	0.0023
1-Ethyl-2-propylbenzene	0.0006
4-methylindane	0.0004
Pentylbenzene	0.0006
Total	1.0000

SD06	
Compound	fraction
Methanol	0.1134
1-Butanol	0.0322
Methy isobutyl ketone	0.1188
Butyl acetate	0.0547
2-Heptanone	0.0220
Diacetone alcohol	0.4314
2,2,4-Trimethyl-1,3-pentanediol	0.2276
Total	1.0000

SD07	
Compound	fraction
2-Pentanone	0.2288
Methyl isobutyl ketone	0.1900
Butyl acetate	0.0445
Exxate 600 (Acetate esters of C6 alcohols)	0.4827
o-Xylene	0.0058
Isopropylbenzene	0.0008
n-propylbenzene	0.0018
1-Methyl-3-ethylbenzene	0.0085
1-Methyl-4-ethylbenzene	0.0038
1,3,5-Trimethylbenzene	0.0054
1-Methyl-2-ethylbenzene	0.0030
1,2,4-Trimethylbenzene	0.0183
s-Butylbenzene	0.0001
i-Butylbenzene	0.0001
1-Methyl-3-isopropylbenzene	0.0002
1,2,3-Trimethylbenzene	0.0034
Indan	0.0004
1,3-Diethylbenzene	0.0001
1-Methyl-3-propylbenzene	0.0003
1-Methyl-4-propylbenzene	0.0006
1-Methyl-2-propylbenzene	0.0001
1,4-Dimethyl-2-ethylbenzene	0.0002
1,4-Dimethyl-2-ethylbenzene	0.0002
1,2-Dimethyl-4-ethylbenzene	0.0004
1,3-Dimethyl-2-ethylbenzene	0.0000
2-Phenyl-2-methylbutane	0.0000
1,2-Dimethyl-3-ethylbenzene	0.0000
1-Ethyl-2-isopropylbenzene	0.0001
1-Ethyl-4-isopropylbenzene	0.0002
1,2,4,5-tetramethylbenzene	0.0002
1-Ethyl-2-propylbenzene	0.0001
4-Methylindane	0.0000
Pentylbenzene	0.0001
Total	1.0000

SD08	
Compound	fraction
Butyl Acetate	1.0000
Total	1.0000

SD09	
Compound	fraction
1-Butanol	1.0000
Total	1.0000

SD10	
Compound	fraction
2-Heptanone	0.9377
Ethylbenzene	0.0085
m-Xylene	0.0245
p-Xylene	0.0088
o-Xylene	0.0205
Total	1.0000

SD11	
Compound	Fraction
toluene	0.0018
3-methylheptane	0.0020
octane	0.0015
cis, cis-1,3,5-trimethylcyclohexane	0.0016
1,1,3-trimethylcyclohexane	0.0028
ethylbenzene	0.0055
trans, trans-1,3,5-trimethylcyclohexane	0.0061
trans, trans-1,2,4-trimethylcyclohexane	0.0014
m-xylene	0.0153
p-xylene	0.0053
4-methyloctane	0.0025
3-methyloctane	0.0032
styrene	0.0016
trans, cis-1,2,4-trimethylcyclohexane	0.0036
1,2,3-trimethylcyclohexane	0.0075
o-xylene	0.0166
1,1,2-trimethylcyclohexane	0.0020
1-methyl-2-propylcyclopentane	0.0035
cis-1-ethyl-3-methylcyclohexane	0.0019
cis-1-ethyl-3-methylcyclohexane	0.0072
trans-1-ethyl-3-methylcyclohexane	0.0045
OTHER C9	0.0014
nonane	0.0184
OTHER C10	0.0036
cis, trans-1,2,3-trimethylcyclohexane	0.0040
trans-1-ethyl-4-methylcyclohexane	0.0112
cis-1-ethyl-4-methylcyclohexane	0.0024
isopropylbenzene	0.0056
3,4-dimethyloctane	0.0034
OTHER C10	0.0019
isopropylcyclohexane	0.0119
2,5-dimethyloctane	0.0037
2,7-dimethyloctane	0.0037
propylcyclohexane	0.0168
2,6-dimethyloctane	0.0155
3,6-dimethyloctane	0.0068
OTHER C10	0.0041
4,5-dimethyloctane	0.0103
propylbenzene	0.0166
4-ethyloctane	0.0039
1-ethyl-3-methylbenzene	0.0488
1-ethyl-4-methylbenzene	0.0300
1,3,5-trimethylbenzene	0.0475
1,1,2,3-tetramethylcyclohexane	0.0100
2-methylnonane	0.0152
OTHER C10	0.0060
1-ethyl-2-methylbenzene	0.0272
1-methyl-4-isopropylcyclohexane	0.0033
1-methyl-3-isopropylcyclohexane	0.0092
1-methyl-3-isopropylcyclohexane	0.0082
1-methyl-4-isopropylcyclohexane	0.0041
diethylcyclohexane	0.0101
1,2,4-trimethylbenzene	0.1227
1-methyl-2-isopropylcyclohexane	0.0108
diethylcyclohexane	0.0051
diethylcyclohexane	0.0037
decane	0.0477
methyl propylcyclohexane	0.0036
sec-butylbenzene	0.0064
methyl propylcyclohexane	0.0056
methyl propylcyclohexane	0.0017
OTHER C11	0.0013
2,4-dimethylnonane	0.0022
2,4-dimethylnonane	0.0059
1,2,3-trimethylbenzene	0.0300
1-methyl-4-isopropylbenzene	0.0066
2,6-dimethylnonane	0.0176
methyl propylcyclohexane	0.0024
indane	0.0070
3,6-dimethylnonane	0.0032
2,7-dimethylnonane	0.0062
butylcyclohexane	0.0054
pentylcyclopentane	0.0106
3,7-dimethylnonane	0.0072
1-methyl-3-propylbenzene	0.0032
5-methylindane	0.0075
1-methyl-4-propylbenzene	0.0093
4-ethylnonane	0.0035
OTHER C11	0.0020
5-methyldecane	0.0068
3-ethylnonane	0.0042
4-methyldecane	0.0053
trans-decalin	0.0072
5-isopropylnonane	0.0019
1-ethyl-2,2,6-trimethylcyclohexane	0.0114
3-methyldecane	0.0099
ethyl propylcyclohexane	0.0022
ethyl propylcyclohexane	0.0033
1,3-dimethyl-2-ethylbenzene	0.0072
methylindane	0.0054
ethyl propylcyclohexane	0.0027
methyl butylcyclohexane	0.0105
cis-decalin	0.0023
ethyl propylcyclohexane	0.0016
undecane	0.0304
2,4-dimethyldecane	0.0089
2-methyldecalin	0.0048
OTHER C12	0.0021
1,2,4,5-tetramethylbenzene	0.0038
2,6-dimethyldecane	0.0071
2,5-dimethyldecane	0.0040
2,7-dimethyldecane	0.0093
OTHER C12	0.0012
OTHER C12	0.0012
OTHER C12	0.0029
pentylcyclohexane	0.0051
methylindane	0.0059
4-ethyldecane	0.0015
6-methylundecane	0.0056
4-methylundecane	0.0026
2-methylundecane	0.0048
3-methylundecane	0.0035
naphthalene	0.0017
dodecane	0.0089
2,6-dimethylundecane	0.0025
Total	1.0000
Fraction Identified	0.9722

SD12	
Compound	Fraction
toluene	0.0009
cis-1,3-dimethylcyclohexane	0.0006
butyl acetate	0.0079
octane	0.0013
cis-1,2-dimethylcyclohexane	0.0008
cis, cis-1,3,5-trimethylcyclohexane	0.0025
ethylcyclohexane	0.0009
1,1,3-trimethylcyclohexane	0.0019
ethylbenzene	0.0050
trans, trans-1,2,4-trimethylcyclohexane	0.0085
2,3-dimethylheptane	0.0011
trans, trans-1,3,5-trimethylcyclohexane	0.0014
m-xylene	0.0146
p-xylene	0.0052
4-methyloctane	0.0027
3-methyloctane	0.0023
trans, cis-1,2,4-trimethylcyclohexane	0.0086
o-xylene	0.0122
cis, trans-1,2,4-trimethylcyclohexane	0.0051
OTHER C9	0.0009
cis-1-ethyl-3-methylcyclohexane	0.0103
cis, cis-1,2,4-trimethylcyclohexane	0.0057
nonane	0.0136
OTHER C10	0.0020
cis, trans-1,2,3-trimethylcyclohexane	0.0055
trans-1-ethyl-4-methylcyclohexane	0.0174
cis-1-ethyl-4-methylcyclohexane	0.0041
isopropylbenzene	0.0021
3,4-dimethyloctane	0.0067
trans-bicyclo[4.3.0]nonane	0.0032
isopropylcyclohexane	0.0104
3,5-dimethyloctane	0.0078
2,5-dimethyloctane	0.0019
cis-1-ethyl-2-methylcyclohexane	0.0071
propylcyclohexane	0.0307
2,6-dimethyloctane	0.0258
butylcyclohexane	0.0116
3,6-dimethyloctane	0.0081
1,1,2,3-tetramethylcyclohexane	0.0213
1,1,3,5-tetramethylcyclohexane	0.0080
2,3-dimethyloctane	0.0048
1-ethyl-3-methylbenzene	0.0073
1-ethyl-4-methylbenzene	0.0096
4-ethyloctane	0.0274
1,3,5-trimethylbenzene	0.0151
4-methylnonane	0.0276
2-methylnonane	0.0258
1-ethyl-1,3-dimethylcyclohexane	0.0197
3-methylnonane	0.0117
1-ethyl-2-methylbenzene	0.0244
OTHER C10	0.0018
1-methyl-4-isopropylcyclohexane	0.0041
1-methyl-3-isopropylcyclohexane	0.0177
methyl isopropylcyclohexane	0.0115
1-ethyl-2,4-dimethylcyclohexane	0.0100
diethylcyclohexane	0.0062
1,2,4-trimethylbenzene	0.0401
diethylcyclohexane	0.0206
cis-bicyclo[4.3.0]nonane	0.0082
methyl propylcyclohexane	0.0058
decane	0.1017
methyl isopropylcyclohexane	0.0063
methyl propylcyclohexane	0.0104
diethylcyclohexane	0.0096
methyl propylcyclohexane	0.0041
2-ethyl-1,3-dimethylcyclohexane	0.0033
2,4-dimethylnonane	0.0145
1,2,3-trimethylbenzene	0.0105
2,5-dimethylnonane	0.0108
2,6-dimethylnonane	0.0261
5-ethyl-3-methyloctane	0.0162
isobutylcyclohexane	0.0091
pentylcyclohexane	0.0079
pentylcyclopentane	0.0170
3,7-dimethylnonane	0.0098
4,5-dimethylnonane	0.0034
5-methylindane	0.0076
4-ethylnonane	0.0067
OTHER C11	0.0048
3-ethylnonane	0.0033
5-methyldecane	0.0090
4-methyldecane	0.0098
trans-decalin	0.0080
OTHER C11	0.0037
3-methyldecane	0.0196
ethyl propylcyclohexane	0.0029
OTHER C11	0.0018
OTHER C11	0.0021
ethyl propylcyclohexane	0.0039
OTHER C11	0.0015
cis-decalin	0.0074
OTHER C11	0.0015
undecane	0.0249
OTHER C12	0.0013
2-methyldecalin	0.0049
2,4-dimethyldecane	0.0033
OTHER C12	0.0011
2,6-dimethyldecane	0.0044
2,5-dimethyldecane	0.0017
2-methyldecalin	0.0010
3,7-dimethyldecane	0.0041
OTHER C12	0.0006
OTHER C12	0.0009
pentylcyclohexane	0.0025
4-ethyldecane	0.0017
5-methylundecane	0.0016
4-methylundecane	0.0008
2-methylundecane	0.0011
3-methylundecane	0.0011
dodecane	0.0013
Total	1.0000
Fraction Identified	0.9768

SD13	
Compound	Fraction
2-methylpentane	0.0010
4-methylheptane	0.0010
cis-1,3-dimethylcyclohexane	0.0011
octane	0.0024
cis, cis-1,3,5-trimethylcyclohexane	0.0009
ethylcyclohexane	0.0013
propylcyclopentane	0.0009
1,1,3-trimethylcyclohexane	0.0015
ethylbenzene	0.0054
trans, trans-1,2,4-trimethylcyclohexane	0.0059
m-xylene	0.0154
p-xylene	0.0059
2-methyloctane	0.0023
3-methyloctane	0.0019
trans, cis-1,2,4-trimethylcyclohexane	0.0064
o-xylene	0.0093
cis, trans-1,2,4-trimethylcyclohexane	0.0037
OTHER C9	0.0009
cis-1-ethyl-3-methylcyclohexane	0.0081
trans-1-ethyl-3-methylcyclohexane	0.0043
nonane	0.0146
OTHER C10	0.0014
cis, trans-1,2,3-trimethylcyclohexane	0.0043
trans-1-ethyl-4-methylcyclohexane	0.0133
cis-1-ethyl-4-methylcyclohexane	0.0030
isopropylbenzene	0.0016
2,4,5-trimethylheptane	0.0059
bicyclo[3.3.0]octane	0.0101
2,5-dimethyloctane	0.0066
3,5-dimethyloctane	0.0015
trans-bicyclo[4.3.0]nonane	0.0061
propylcyclohexane	0.0239
2,6-dimethyloctane	0.0209
2,2,3,3-tetramethylhexane	0.0094
3,6-dimethyloctane	0.0065
1-ethyl-2,4-dimethylcyclohexane	0.0163
3-ethyl-2-methylheptane	0.0054
propylbenzene	0.0036
OTHER C10	0.0051
1-ethyl-3-methylbenzene	0.0064
1-ethyl-4-methylbenzene	0.0215
1,3,5-trimethylbenzene	0.0132
5-methylnonane	0.0233
4-methylnonane	0.0250
2-methylnonane	0.0138
1-ethyl-1,3-dimethylcyclohexane	0.0096
3-methylnonane	0.0215
1-ethyl-2-methylbenzene	0.0011
1-methyl-4-isopropylcyclohexane	0.0028
1-methyl-3-isopropylcyclohexane	0.0138
OTHER C9	0.0087
1-methyl-4-isopropylcyclohexane	0.0083
1-ethyl-1,2-dimethylcyclohexane	0.0047
1,2,4-trimethylbenzene	0.0330
1-methyl-2-isopropylcyclohexane	0.0172
1-methyl-2-isopropylcyclohexane	0.0066
2-ethyl-1,3-dimethylcyclohexane	0.0045
decane	0.1074
methyl propylcyclohexane	0.0086
diethylcyclohexane	0.0081
methyl propylcyclohexane	0.0031
OTHER C11	0.0029
OTHER C11	0.0014
1-methyl-3-isopropylbenzene	0.0119
1,2,3-trimethylbenzene	0.0080
OTHER C11	0.0105
2,5-dimethylnonane	0.0274
2,4,6-trimethyloctane	0.0025
methyl propylcyclohexane	0.0125
methyl propylcyclohexane	0.0076
isobutylcyclohexane	0.0079
butylcyclohexane	0.0177
2,7-dimethylnonane	0.0098
3,7-dimethylnonane	0.0030
methyl propylcyclohexane	0.0075
butylbenzene	0.0064
1-ethyl-2,2,6-trimethylcyclohexane	0.0054
5-ethyl-2-methyloctane	0.0034
5-methyldecane	0.0120
4-methyldecane	0.0123
trans-decalin	0.0117
2-methyldecane	0.0153
3-methyldecane	0.0134
ethyl propylcyclohexane	0.0031
ethyl propylcyclohexane	0.0027
ethyl propylcyclohexane	0.0022
ethyl propylcyclohexane	0.0045
methyl butylcyclohexane	0.0021
methyl butylcyclohexane	0.0108
methyl butylcyclohexane	0.0023
methyl butylcyclohexane	0.0022
undecane	0.0577
1-ethyl-4-isopropylbenzene	0.0084
diethylcyclohexane	0.0060
ethyl propylcyclohexane	0.0021
2,5-dimethyldecane	0.0086
2,6-dimethyldecane	0.0029
2-methyldecalin	0.0026
3-ethyl-2-methyloctane	0.0093
5-sec butylnonane	0.0008
OTHER C12	0.0016
OTHER C12	0.0022
pentylcyclohexane	0.0072
3-ethyldecane	0.0040
2,3-dimethyldecane	0.0014
6-methylundecane	0.0036
5-methylundecane	0.0028
4-methylundecane	0.0047
2-methylundecane	0.0053
3-methylundecane	0.0046
OTHER C12	0.0009
OTHER C12	0.0016
dodecane	0.0154
OTHER C13	0.0014
1,1,5-trimethylindane	0.0016
2,6-dimethylundecane	0.0022
Total	1.0000
fraction Identified	0.9616

SD14	
Compound	Fraction
butyl alcohol	0.0011
3-methylhexane	0.0077
2,4-dimethylpentane	0.0031
1,1-dimethylcyclopentane	0.0015
2-methylhexane	0.0200
cis-1,3-dimethylcyclopentane	0.0104
trans-1,3-dimethylcyclopentane	0.0146
1,2-dimethylcyclopentane	0.0236
heptane	0.1859
1,2-dimethylcyclopentane	0.0118
methylcyclohexane	0.4104
1,1,3-trimethylcyclopentane	0.0261
2,4-dimethylhexane	0.0165
ethylcyclopentane	0.0150
1,2,4-trimethylcyclopentane	0.0233
1,2,4-trimethylcyclopentane	0.0286
1,2,3-trimethylcyclopentane	0.0205
2,3,4-trimethylpentane	0.0026
toluene	0.0053
2,3-dimethylhexane	0.0085
3-ethyl-2-methylpentane	0.0023
1,1,2-trimethylcyclopentane	0.0063
2-methylheptane	0.0449
4-methylheptane	0.0122
3,4-dimethylhexane	0.0030
3-methylheptane	0.0226
3-ethylhexane	0.0079
cis-1,3-dimethylcyclohexane	0.0233
trans-1,4-dimethylcyclohexane	0.0078
1,1-dimethylcyclohexane	0.0030
cis-1-ethyl-3-methylcyclopentane	0.0011
trans-1-ethyl-3-methylcyclopentane	0.0010
cis-1-ethyl-2-methylcyclopentane	0.0017
trans-1,2-dimethylcyclohexane	0.0009
octane	0.0110
cis-1,4-dimethylcyclohexane	0.0037
cis-1,2-dimethylcyclohexane	0.0012
cis, cis-1,3,5-trimethylcyclohexane	0.0008
ethylcyclohexane	0.0016
2,5-dimethylheptane	0.0005
1,1,3-trimethylcyclohexane	0.0009
trans, trans-1,2,4-trimethylcyclohexane	0.0015
trans, trans-1,3,5-trimethylcyclohexane	0.0006
4-methyloctane	0.0008
1,2,3-trimethylcyclohexane	0.0018
styrene	0.0008
Total	1.0000
Fraction Identified	1.0000

SD15	
Compound	Fraction
methanol	0.0183
ethanol	0.1183
acetone	0.1739
2-methylbutane	0.0002
methyl ethyl ketone	0.0006
methylcyclopentane	0.0005
OTHER C7	0.0002
2,4-dimethylpentane	0.0007
cyclohexane	0.0082
2-methylhexane	0.0185
2,3-dimethylpentane	0.0082
1,1-dimethylcyclopentane	0.0033
2-methylhexane	0.0259
cis-1,3-dimethylcyclopentane	0.0101
trans-1,3-dimethylcyclopentane	0.0125
1,2-dimethylcyclopentane	0.0188
heptane	0.0655
methyl isobutyl ketone	0.0013
1,2-dimethylcyclopentane	0.0035
methylcyclohexane	0.0720
1,1,3-trimethylcyclopentane	0.0055
2,4-dimethylhexane	0.0030
ethylcyclopentane	0.0127
1,2,4-trimethylcyclopentane	0.0075
1,2,3-trimethylcyclopentane	0.0084
2,3,4-trimethylpentane	0.0010
toluene	0.1921
2,3-dimethylhexane	0.0013
3-ethyl-2methylpentane	0.0006
1,1,2-trimethylcyclopentane	0.0011
2-methylheptane	0.0062
4-methylheptane	0.0015
3,4-dimethylhexane	0.0003
3-methylheptane	0.0019
3-ethylhexane	0.0006
cis-1,3-dimethylcyclohexane	0.0017
trans-1,4-dimethylcyclohexane	0.0006
1,1-dimethylcyclohexane	0.0002
cis-1-ethyl-2-methylcyclopentane	0.0003
butyl acetate	0.0570
octane	0.0003
ethylbenzene	0.0126
m-xylene	0.0353
p-xylene	0.0128
methyl amyl ketone	0.0429
o-xylene	0.0081
2-butoxyethanol	0.0239
Total	1.0000
Fraction Identified	0.9998

SD16	
Compound	Fraction
2,3-dimethylpentane	0.0005
heptane	0.0026
1,2,4-trimethylcyclopentane	0.0018
toluene	0.0009
2-methylheptane	0.0007
3-methylheptane	0.0019
cis-1,3-dimethylcyclohexane	0.0009
octane	0.0051
trans-1,3-dimethylcyclohexane	0.0008
2,4-dimethylheptane	0.0004
cis-1,2-dimethylcyclohexane	0.0016
ethylcyclohexane	0.0037
2,5-dimethylheptane	0.0013
1,1,3-trimethylcyclohexane	0.0013
1,1,4-trimethylcyclohexane	0.0005
ethylbenzene	0.0020
trans, trans-1,2,4-trimethylcyclohexane	0.0014
2,3-dimethylheptane	0.0013
m-xylene	0.0151
4-methyloctane	0.0053
cis-bicyclo[3.3.0]octane	0.0006
3-ethylheptane	0.0038
trans, cis-1,2,4-trimethylcyclohexane	0.0013
o-xylene	0.0062
1,2,3-trimethylcyclohexane	0.0016
diethylcyclohexane	0.0004
cis-1-ethyl-3-methylcyclohexane	0.0046
cis, cis-1,2,4-trimethylcyclohexane	0.0024
OTHER C9	0.0007
nonane	0.0271
trans-1-ethyl-2-methylcyclohexane	0.0011
trans-1-ethyl-4-methylcyclohexane	0.0041
cis-1-ethyl-4-methylcyclohexane	0.0012
isopropylbenzene	0.0021
3,4-dimethyloctane	0.0029
isopropylcyclohexane	0.0062
3,5-dimethyloctane	0.0031
2,5-dimethyloctane	0.0006
cis-1-ethyl-2-methylcyclohexane	0.0026
2,7-dimethyloctane	0.0011
propylcyclohexane	0.0099
2,6-dimethyloctane	0.0077
3,3,5-trimethylheptane	0.0030
3,6-dimethyloctane	0.0022
4,5-dimethyloctane	0.0044
2,3-dimethyloctane	0.0049
1,1,3,5-tetramethylcyclohexane	0.0011
1,2-dimethyl-3-ethylcyclohexane	0.0020
1-ethyl-3-methylbenzene	0.0129
1-ethyl-4-methylbenzene	0.0121
3-ethyl-4-methylheptane	0.0010
4-methylnonane	0.0287
2-methylnonane	0.0158
3-methylnonane	0.0034
1-ethyl-2-methylbenzene	0.0150
1-methyl-4-isopropylcyclohexane	0.0007
OTHER C10	0.0060
1-methyl-3-isopropylcyclohexane	0.0014
1-methyl-3-isopropylcyclohexane	0.0021
1-ethyl-2,4-dimethylcyclohexane	0.0028
1-methyl-2-isopropylcyclohexane	0.0015
1,2,4-trimethylbenzene	0.0425
cis-bicyclo[4.3.0]nonane	0.0076
1-methyl-2-isopropylcyclohexane	0.0022
1,2-dimethyl-3-ethylcyclohexane	0.0033
decane	0.1026
sec butylbenzene	0.0053
diethylcyclohexane	0.0069
diethylcyclohexane	0.0012
OTHER C11	0.0005
1-methyl-3-isopropylbenzene	0.0104
1,2,3-trimethylbenzene	0.0190
1-methyl-4-isopropylbenzene	0.0027
2,5-dimethylnonane	0.0063
2,6-dimethylnonane	0.0238
3,5-dimethylnonane	0.0015
indane	0.0101
isobutylcyclohexane	0.0070
butylcyclohexane	0.0077
pentylcyclopentane	0.0159
3,7-dimethylnonane	0.0062
1-methyl-3-propylbenzene	0.0049
5-methylindane	0.0141
1-methyl-4-propylbenzene	0.0257
5-methyldecane	0.0150
4-methyldecane	0.0115
2-methyldecane	0.0215
1,2-dimethyl-4-ethylbenzene	0.0170
3-methyldecane	0.0190
1,3-dimethyl-4-ethylbenzene	0.0068
OTHER C11	0.0022
1-methylindane	0.0134
1,3-dimethyl-2-ethylbenzene	0.0069
ethyl propylcyclohexane	0.0041
ethyl propylcyclohexane	0.0085
1-methyl-4-isobutylbenzene	0.0031
undecane	0.1224
ethyl propylcyclohexane	0.0048
1-ethyl-4-isopropylbenzene	0.0076
3-phenylpentane	0.0091
1,2,4,5-tetramethylbenzene	0.0066
1,2,3,5-tetramethylbenzene	0.0144
2,6-dimethyldecane	0.0030
2-methyldecalin	0.0030
OTHER C12	0.0104
1,3-dimethyl-4-isopropylbenzene	0.0024
4,5-dimethyldecane	0.0023
(2-methylbutyl)cyclohexane	0.0063
pentylcyclohexane	0.0075
4-ethyldecane	0.0080
3-ethyldecane	0.0027
6-methylundecane	0.0092
4-methylundecane	0.0041
2-methylundecane	0.0098
3-methylundecane	0.0046
OTHER C12	0.0004
naphthalene	0.0111
1,2,3-trimethyl-4-ethylbenzene	0.0011
dodecane	0.0216
2,6-dimethylundecane	0.0024
hexylcyclohexane	0.0009
OTHER C13	0.0004
OTHER C13	0.0005
OTHER C13	0.0009
tridecane	0.0026
2-methylnaphthalene	0.0021
OTHER C14	0.0008
Total	1.0000
Fraction Identified	0.9773

SD17	
Compound	Fraction
toluene	0.0007
2,3-dimethylhexane	0.0014
2-methylheptane	0.0041
3-methylheptane	0.0010
octane	0.0028
cis, cis-1,3,5-trimethylcyclohexane	0.0016
ethylcyclohexane	0.0016
1,1,3-trimethylcyclohexane	0.0016
2,5-dimethylheptane	0.0010
1,1,3-trimethylcyclohexane	0.0029
ethylbenzene	0.0060
trans, trans-1,2,4-trimethylcyclohexane	0.0059
2,3-dimethylheptane	0.0024
m-xylene	0.0147
p-xylene	0.0056
4-methyloctane	0.0016
2-methyloctane	0.0026
3-methyloctane	0.0040
trans, cis-1,2,4-trimethylcyclohexane	0.0059
o-xylene	0.0120
1,1,2-trimethylcyclohexane	0.0026
1,2,3-trimethylcyclohexane	0.0025
cis-1-ethyl-3-methylcyclohexane	0.0014
diethylcyclohexane	0.0085
cis, cis-1,2,4-trimethylcyclohexane	0.0046
OTHER C9	0.0010
OTHER C9	0.0007
nonane	0.0207
trans-1-ethyl-2-methylcyclohexane	0.0019
cis, trans-1,2,3-trimethylcyclohexane	0.0038
trans-1-ethyl-4-methylcyclohexane	0.0134
cis-1-ethyl-4-methylcyclohexane	0.0033
OTHER C10	0.0012
3,4-dimethyloctane	0.0059
isopropylcyclohexane	0.0117
3,5-dimethyloctane	0.0066
2,5-dimethyloctane	0.0018
cis-1-ethyl-2-methylcyclohexane	0.0052
propylcyclohexane	0.0244
2,6-dimethyloctane	0.0225
3,3,5-trimethylheptane	0.0029
butylcyclohexane	0.0068
3,6-dimethyloctane	0.0065
1,1,2,3-tetramethylcyclohexane	0.0172
3-ethyl-2-methylheptane	0.0060
1,1,3,5-tetramethylcyclohexane	0.0040
1,2-dimethyl-3-ethylcyclohexane	0.0061
1-ethyl-3-methylbenzene	0.0047
1,1,2,3-tetramethylcyclohexane	0.0201
4-ethyloctane	0.0117
4-methylnonane	0.0215
2-methylnonane	0.0362
3-methylnonane	0.0087
1-ethyl-2-methylbenzene	0.0202
OTHER C10	0.0014
1-methyl-4-isopropylcyclohexane	0.0034
1-methyl-4-isopropylcyclohexane	0.0148
1-methyl-3-isopropylcyclohexane	0.0091
1-ethyl-2,4-dimethylcyclohexane	0.0075
1-methyl-2-isopropylcyclohexane	0.0049
1,2,4-trimethylbenzene	0.0299
OTHER C10	0.0164
1-methyl-2-isopropylcyclohexane	0.0120
decane	0.1029
methyl propylcyclohexane	0.0092
methyl propylcyclohexane	0.0088
methyl propylcyclohexane	0.0032
diethylcyclohexane	0.0029
2-ethyl-1,3-dimethylcyclohexane	0.0018
1-methyl-3-isopropylbenzene	0.0130
1,2,3-trimethylbenzene	0.0095
2,5-dimethylnonane	0.0118
2,6-dimethylnonane	0.0288
methyl propylcyclohexane	0.0031
OTHER C11	0.0135
isobutylcyclohexane	0.0094
isopentylcyclohexane	0.0085
pentylcyclopentane	0.0172
3,7-dimethylnonane	0.0117
1,3-diethylbenzene	0.0045
methyl propylcyclohexane	0.0097
4-ethylnonane	0.0098
3-ethylnonane	0.0061
5-methyldecane	0.0031
4-methyldecane	0.0120
2-methyldecane	0.0134
trans-decalin	0.0122
5-isopropylnonane	0.0136
3-methyldecane	0.0139
1,3-dimethyl-4-ethylbenzene	0.0030
1,1-dimethyl-2-propylcyclohexane	0.0032
1-methylindane	0.0029
1,2-dimethyl-4-ethylbenzene	0.0055
1,3-dimethyl-2-ethylbenzene	0.0056
ethyl propylcyclohexane	0.0033
methyl butylcyclohexane	0.0108
OTHER C11	0.0025
undecane	0.0469
1-ethyl-4-isopropylbenzene	0.0033
2-methyldecalin	0.0057
ethyl propylcyclohexane	0.0070
1,2,4,5-tetramethylbenzene	0.0018
1,2,3,5-tetramethylbenzene	0.0086
2,6-dimethyldecane	0.0027
2-methyldecalin	0.0020
3,5-dimethylnonane	0.0067
4,5-dimethylnonane	0.0013
OTHER C12	0.0013
OTHER C12	0.0025
pentylcyclohexane	0.0045
4-ethyldecane	0.0033
3-ethyldecane	0.0011
5-methylundecane	0.0041
4-methylundecane	0.0019
2-methylundecane	0.0027
3-methylundecane	0.0019
dodecane	0.0051
Total	1.0000
Fraction Identified	0.9594

SD18	
Compound	Fraction
methyl ethyl ketone	0.0009
2-methylheptane	0.0007
3,4-dimethylhexane	0.0020
cis-1,3-dimethylcyclohexane	0.0006
trans-1,2-dimethylcyclohexane	0.0005
octane	0.0012
cis-1,2-dimethylcyclohexane	0.0009
cis, cis-1,3,5-trimethylcyclohexane	0.0016
ethylcyclohexane	0.0010
1,1,3-trimethylcyclohexane	0.0023
ethylbenzene	0.0057
trans, trans-1,2,4-trimethylcyclohexane	0.0059
2,3-dimethylheptane	0.0011
OTHER C9	0.0006
m-xylene	0.0141
p-xylene	0.0053
2-methyloctane	0.0025
3-methyloctane	0.0026
OTHER C9	0.0007
trans, cis-1,2,4-trimethylcyclohexane	0.0065
o-xylene	0.0135
cis, trans-1,2,4-trimethylcyclohexane	0.0026
1,2,3-trimethylcyclohexane	0.0018
OTHER C9	0.0014
cis-1-ethyl-3-methylcyclohexane	0.0073
trans-1-ethyl-3-methylcyclohexane	0.0043
nonane	0.0146
trans-1-ethyl-2-methylcyclohexane	0.0024
cis, trans-1,2,3-trimethylcyclohexane	0.0038
trans-1-ethyl-4-methylcyclohexane	0.0117
cis-1-ethyl-4-methylcyclohexane	0.0026
isopropylbenzene	0.0043
3,4-dimethyloctane	0.0040
OTHER C10	0.0020
isopropylcyclohexane	0.0090
3,5-dimethyloctane	0.0047
2,5-dimethyloctane	0.0011
cis-1-ethyl-2-methylcyclohexane	0.0042
propylcyclohexane	0.0189
2,6-dimethyloctane	0.0178
3,3,5-trimethylheptane	0.0023
4,5-dimethyloctane	0.0057
3,6-dimethyloctane	0.0051
1,1,2,3-tetramethylcyclohexane	0.0129
1,1,3,5-tetramethylcyclohexane	0.0154
1,2-dimethyl-3-ethylcyclohexane	0.0044
1-ethyl-3-methylbenzene	0.0374
1,1,2,3-tetramethylcyclohexane	0.0285
4-methylnonane	0.0456
2-methylnonane	0.0138
1-ethyl-1,3-dimethylcyclohexane	0.0153
3-methylnonane	0.0070
1-ethyl-2-methylbenzene	0.0137
1-ethyl-2,4-dimethylcyclohexane	0.0136
1-methyl-4-isopropylcyclohexane	0.0029
1-methyl-3-isopropylcyclohexane	0.0105
1-methyl-3-isopropylcyclohexane	0.0079
1-ethyl-2,4-dimethylcyclohexane	0.0062
diethylcyclohexane	0.0037
1,2,4-trimethylbenzene	0.0797
1-methyl-2-isopropylcyclohexane	0.0129
1-methyl-2-isopropylcyclohexane	0.0094
decane	0.0646
sec butylbenzene	0.0044
diethylcyclohexane	0.0073
methyl propylcyclohexane	0.0065
methyl propylcyclohexane	0.0023
OTHER C11	0.0019
OTHER C11	0.0018
2,4-dimethylnonane	0.0078
1,2,3-trimethylbenzene	0.0204
2,5-dimethylnonane	0.0080
2,6-dimethylnonane	0.0225
5-ethyl-3-methyloctane	0.0114
isobutylcyclohexane	0.0084
butylcyclohexane	0.0061
pentylcyclopentane	0.0135
3,7-dimethylnonane	0.0081
1,3-diethylbenzene	0.0033
4-ethylnonane	0.0078
trans-decalin	0.0090
OTHER C11	0.0040
3-ethylnonane	0.0024
5-methyldecane	0.0089
4-methyldecane	0.0113
2-methyldecane	0.0096
diethylcyclohexane	0.0135
3-methyldecane	0.0121
ethyl propylcyclohexane	0.0034
ethyl propylcyclohexane	0.0030
1,2-dimethyl-4-ethylbenzene	0.0056
1,3-dimethyl-2-ethylbenzene	0.0055
ethyl propylcyclohexane	0.0032
cis-decalin	0.0127
ethyl propylcyclohexane	0.0026
1-ethyl-2-isopropylcyclohexane	0.0020
undecane	0.0517
2-methyldecalin	0.0104
2,4-dimethyldecane	0.0067
OTHER C12	0.0021
1,2,4,5-tetramethylbenzene	0.0018
1,2,3,5-tetramethylbenzene	0.0097
2-methyldecalin	0.0026
3,7-dimethyldecane	0.0106
4,5-dimethyldecane	0.0014
OTHER C12	0.0016
(2-methylbutyl)cyclohexane	0.0027
pentylcyclohexane	0.0065
4-ethyldecane	0.0051
3-ethyldecane	0.0015
5-methylundecane	0.0062
4-methylundecane	0.0031
2-methylundecane	0.0046
3-methylundecane	0.0035
OTHER C12	0.0006
naphthalene	0.0006
dodecane	0.0084
2,6-dimethylundecane	0.0018
Total	1.0000
Fraction Identified	0.9860

SD19	
Compound	Fraction
methylcyclohexane	0.0058
1,1,3-trimethylcyclopentane	0.0015
2,5-dimethylhexane	0.0015
2,4-dimethylhexane	0.0028
1,2,4-trimethylcyclopentane	0.0055
1,2,3-trimethylcyclopentane	0.0052
2,3,4-trimethylpentane	0.0011
toluene	0.0090
2,3-dimethylhexane	0.0061
3-ethyl-2-methylpentane	0.0018
1,1,2-trimethylcyclopentane	0.0037
2-methylheptane	0.0553
4-methylheptane	0.0159
3,4-dimethylhexane	0.0041
3-methylheptane	0.0415
3-ethylhexane	0.0074
cis-1,3-dimethylcyclohexane	0.0941
trans-1,4-dimethylcyclohexane	0.0343
OTHER OTHER C8	0.0017
1,1-dimethylcyclohexane	0.0100
1-ethyl-3-methylcyclopentane	0.0044
1-ethyl-3-methylcyclopentane	0.0043
1-ethyl-2-methylcyclopentane	0.0083
trans-1,2-dimethylcyclohexane	0.0028
octane	0.1702
cis-1,4-dimethylcyclohexane	0.0045
trans-1,3-dimethylcyclohexane	0.0403
1-ethyl-1-methylcyclopentane	0.0033
OTHER C9	0.0023
2,2-dimethylheptane	0.0015
2,2,5-trimethylhexane	0.0060
2,4-dimethylheptane	0.0110
OTHER C9	0.0008
cis-1,2-dimethylcyclohexane	0.0020
2,6-dimethylheptane	0.0355
propylcyclopentane	0.0039
cis, cis-1,3,5-trimethylcyclohexane	0.0338
ethylcyclohexane	0.0447
2,5-dimethylheptane	0.0179
OTHER C9	0.0022
1,1,3-trimethylcyclohexane	0.0294
1,1,4-trimethylcyclohexane	0.0069
OTHER C9	0.0014
2,6-dimethyloctane	0.0035
OTHER C9	0.0016
ethylbenzene	0.0059
trans, trans-1,2,4-trimethylcyclohexane	0.0576
trans, trans-1,3,5-trimethylcyclohexane	0.0272
m-xylene	0.0038
p-xylene	0.0020
2,3-dimethyloctane	0.0024
4-methyloctane	0.0114
2-methyloctane	0.0155
cis-bicyclo[3.3.0]octane	0.0018
3-ethylheptane	0.0045
3-methyloctane	0.0159
OTHER C9	0.0012
1,2,3-trimethylcyclohexane	0.0007
trans, cis-1,2,4-trimethylcyclohexane	0.0313
1,2,3-trimethylcyclohexane	0.0120
cis, trans-1,2,4-trimethylcyclohexane	0.0139
cis-1-ethyl-3-methylcyclohexane	0.0157
trans-1-ethyl-3-methylcyclohexane	0.0069
cis, cis-1,2,4-trimethylcyclohexane	0.0014
nonane	0.0078
cis, trans-1,2,3-trimethylcyclohexane	0.0030
trans-1-ethyl-2-methylcyclohexane	0.0055
isopropylcyclohexane	0.0020
Total	1.0000
Fraction Identified	0.9888

SD21	
Compound	Fraction
heptane	0.0011
methylcyclohexane	0.0018
2-methylheptane	0.0018
4-methylheptane	0.0005
3-methylheptane	0.0011
cis-1,3-dimethylcyclohexane	0.0021
cis-1,3-dimethylcyclohexane	0.0008
octane	0.0062
trans-1,3-dimethylcyclohexane	0.0007
2,6-dimethylheptane	0.0027
ethylcyclohexane	0.0006
2,5-dimethylheptane	0.0024
1,1,3-trimethylcyclohexane	0.0011
OTHER C9	0.0051
ethylbenzene	0.0013
trans, trans-1,3,5-trimethylcyclohexane	0.0039
m-xylene	0.0019
p-xylene	0.0026
4-methyloctane	0.0048
3-methyloctane	0.0041
trans, cis-1,2,4-trimethylcyclohexane	0.0007
1,2,3-trimethylcyclohexane	0.0037
o-xylene	0.0017
1,1,2-trimethylcyclohexane	0.0036
cis-1-ethyl-3-methylcyclohexane	0.0017
trans-1-ethyl-3-methylcyclohexane	0.0044
cis, cis-1,2,4-trimethylcyclohexane	0.0027
nonane	0.0237
OTHER C10	0.0021
cis, trans-1,2,3-trimethylcyclohexane	0.0017
trans-1-ethyl-4-methylcyclohexane	0.0062
cis-1-ethyl-4-methylcyclohexane	0.0013
2,4-dimethyloctane	0.0007
3,4-dimethyloctane	0.0026
2,3,5-trimethylheptane	0.0012
isopropylcyclohexane	0.0061
3,5-dimethyloctane	0.0030
2,5-dimethyloctane	0.0006
2,7-dimethyloctane	0.0027
propylcyclohexane	0.0114
2,6-dimethyloctane	0.0157
2,2,3,3-tetramethylpentane	0.0022
4,5-dimethyloctane	0.0049
3,6-dimethyloctane	0.0040
3-ethyl-2-methylheptane	0.0095
1,2-dimethyl-3-ethylcyclohexane	0.0033
propylbenzene	0.0023
1,1,2,3-tetramethylcyclohexane	0.0029
1-ethyl-3-methylbenzene	0.0036
1-ethyl-4-methylbenzene	0.0102
1,3,5-trimethylbenzene	0.0058
4-methylnonane	0.0184
2-methylnonane	0.0123
2,3-dimethyloctan	0.0171
3-ethyloctane	0.0055
3-methylnonane	0.0133
1-ethyl-2-methylbenzene	0.0033
1-methyl-3-isopropylcyclohexane	0.0075
1-methyl-3-isopropylcyclohexane	0.0065
2-ethyl-1,3-dimethylcyclohexane	0.0053
1-ethyl-1,2-dimethylcyclohexane	0.0033
1,2,4-trimethylbenzene	0.0266
1-methyl-2-isopropylcyclohexane	0.0123
1,1,3,4-tetramethylcyclohexane	0.0092
decane	0.1145
methyl propylcyclohexane	0.0091
methyl propylcyclohexane	0.0061
diethylcyclohexane	0.0020
diethylcyclohexane	0.0014
2,4-dimethylnonane	0.0028
1-methyl-3-isopropylbenzene	0.0101
1,2,3-trimethylbenzene	0.0125
2,5-dimethylnonane	0.0123
2,6-dimethylnonane	0.0461
methyl propylcyclohexane	0.0030
methyl propylcyclohexane	0.0125
isobutylcyclohexane	0.0080
methyl propylcyclohexane	0.0104
butylcyclohexane	0.0213
3,7-dimethylnonane	0.0157
1-methyl-3-propylbenzene	0.0053
5-methylindane	0.0120
1,3-dimethyl-5-ethylbenzene	0.0128
3-ethyl-3-methyloctane	0.0071
1-ethyl-2,2,6-trimethylcyclohexane	0.0039
5-methyldecane	0.0166
4-methyldecane	0.0203
2-methyldecane	0.0198
5-isopropylnonane	0.0053
1,4-dimethyl-2-ethylbenzene	0.0103
3-methyldecane	0.0188
1,1-dimethyl-2-propylcyclohexane	0.0038
OTHER C11	0.0044
1,3-dimethyl-2-ethylbenzene	0.0060
1-methylindane	0.0069
1,2-diethyl-1-methylcyclohexane	0.0064
ethyl propylcyclohexane	0.0056
ethyl propylcyclohexane	0.0197
cis-decalin	0.0029
undecane	0.1011
ethyl propylcyclohexane	0.0041
ethyl propylcyclohexane	0.0081
OTHER C12	0.0071
1,2,4,5-tetramethylbenzene	0.0046
2,6-dimethyldecane	0.0098
2-methyldecalin	0.0041
6-ethyl-2-methyloctane	0.0089
2,7-dimethyldecane	0.0016
1-methyl-3-butylbenzene	0.0014
pentylcyclohexane	0.0030
hexylcyclopentane	0.0056
4-methylindane	0.0046
OTHER C12	0.0014
5-methylundecane	0.0057
4-methylundecane	0.0021
2-methylundecane	0.0049
3-methylundecane	0.0019
naphthalene	0.0014
methyl pentylcyclohexane	0.0006
dodecane	0.0068
2,6-dimethylundecane	0.0021
Total	1.0000
Fraction Identified	0.9799

SD22	
Compound	Fraction
2-methylheptane	0.0016
3,4-dimethylhexane	0.0047
cis-1,3-dimethylcyclohexane	0.0010
octane	0.0023
cis-1,2-dimethylcyclohexane	0.0014
cis, cis-1,3,5-trimethylcyclohexane	0.0010
ethylcyclohexane	0.0013
1,1,3-trimethylcyclohexane	0.0029
ethylbenzene	0.0081
trans, trans-1,2,4-trimethylcyclohexane	0.0045
2,3-dimethylheptane	0.0020
m-xylene	0.0214
p-xylene	0.0084
2-methyloctane	0.0037
3-methyloctane	0.0036
trans, cis-1,2,4-trimethylcyclohexane	0.0010
trans, cis-1,2,4-trimethylcyclohexane	0.0053
o-xylene	0.0157
1,1,2-trimethylcyclohexane	0.0050
OTHER C9	0.0019
cis-1-ethyl-3-methylcyclohexane	0.0067
cis, cis-1,2,4-trimethylcyclohexane	0.0041
OTHER C9	0.0014
OTHER C9	0.0008
nonane	0.0201
trans-1-ethyl-2-methylcyclohexane	0.0034
cis, trans-1,2,3-trimethylcyclohexane	0.0033
trans-1-ethyl-4-methylcyclohexane	0.0106
cis-1-ethyl-4-methylcyclohexane	0.0023
2,4-dimethyloctane	0.0009
OTHER C10	0.0011
3,4-dimethyloctane	0.0037
isopropylcyclohexane	0.0127
3,5-dimethyloctane	0.0042
2,5-dimethyloctane	0.0010
2,7-dimethyloctane	0.0038
propylcyclohexane	0.0179
2,6-dimethyloctane	0.0179
3,3,5-trimethylheptane	0.0027
4,5-dimethyloctane	0.0054
3,6-dimethyloctane	0.0047
3-ethyl-2-methylheptane	0.0123
1,2-dimethyl-3-ethylcyclohexane	0.0061
propylbenzene	0.0028
1,2-dimethyl-3-ethylcyclohexane	0.0048
1-ethyl-3-methylbenzene	0.0084
1-ethyl-4-methylbenzene	0.0142
1-ethyl-4-methylbenzene	0.0039
4-methylnonane	0.0231
2-methylnonane	0.0122
1,3,5-trimethylbenzene	0.0186
3-methylnonane	0.0072
1-ethyl-2-methylbenzene	0.0150
1-methyl-4-isopropylcyclohexane	0.0052
1-methyl-3-isopropylcyclohexane	0.0121
1-methyl-3-isopropylcyclohexane	0.0103
1-ethyl-2,4-dimethylcyclohexane	0.0073
1-ethyl-1,2-dimethylcyclohexane	0.0048
1,2,4-trimethylbenzene	0.0340
1-methyl-2-isopropylcyclohexane	0.0143
1,1,3,4-tetramethylcyclohexane	0.0120
decane	0.0692
diethylcyclohexane	0.0051
methyl propylcyclohexane	0.0084
methyl propylcyclohexane	0.0076
methyl propylcyclohexane	0.0026
2,4-dimethylnonane	0.0054
1,2,3-trimethylbenzene	0.0249
2,5-dimethylnonane	0.0121
2,6-dimethylnonane	0.0284
methyl propylcyclohexane	0.0037
methyl propylcyclohexane	0.0115
isobutylcyclohexane	0.0103
butylcyclohexane	0.0083
pentylcyclopentane	0.0150
3,7-dimethylnonane	0.0119
1,3-diethylbenzene	0.0046
5-methylindane	0.0105
1,3-dimethyl-5-ethylbenzene	0.0123
3-ethyl-3-methyloctane	0.0058
5-methyldecane	0.0142
3-ethylnonane	0.0060
4-methyldecane	0.0081
2-methyldecane	0.0115
5-isopropylnonane	0.0022
1,4-dimethyl-2-ethylbenzene	0.0141
3-methyldecane	0.0143
1,3-dimethyl-4-ethylbenzene	0.0037
OTHER C11	0.0043
1-methylindane	0.0037
1,2-dimethyl-4-ethylbenzene	0.0065
1,3-dimethyl-2-ethylbenzene	0.0075
ethyl propylcyclohexane	0.0046
ethyl propylcyclohexane	0.0141
cis-decalin	0.0033
undecane	0.0498
1-ethyl-4-isopropylbenzene	0.0042
2-methyldecalin	0.0071
ethyl propylcyclohexane	0.0049
1,2,4,5-tetramethylbenzene	0.0045
1,2,4,5-tetramethylbenzene	0.0043
2,6-dimethyldecane	0.0102
3,5-dimethyldecane	0.0035
2-methyldecalin	0.0020
3-methylnonane	0.0110
2,7-dimethyldecane	0.0023
1-methyl-3-butylbenzene	0.0019
(2-methylbutyl)cyclohexane	0.0045
pentylcyclohexane	0.0059
4-methylindane	0.0075
4-ethyldecane	0.0022
5-methylundecane	0.0078
4-methylundecane	0.0036
2-methylundecane	0.0065
3-methylundecane	0.0046
OTHER C12	0.0011
OTHER C12	0.0009
naphthalene	0.0027
OTHER C12	0.0010
methyl pentylcyclohexane	0.0015
OTHER C12	0.0010
dodecane	0.0123
2,6-dimethylundecane	0.0023
Total	1.0000
Fraction Identified	0.9866

SD23	
Compound	Fraction
2,3,4-trimethylpentane	0.0024
3,4-dimethylhexane	0.0016
octane	0.0017
cis, cis-1,3,5-trimethylcyclohexane	0.0018
1,1,3-trimethylcyclohexane	0.0021
ethylbenzene	0.0072
trans, trans-1,2,4-trimethylcyclohexane	0.0067
2,3-dimethylheptane	0.0022
m-xylene	0.0197
p-xylene	0.0075
2-methyloctane	0.0036
3-methyloctane	0.0034
trans, cis-1,2,4-trimethylcyclohexane	0.0071
o-xylene	0.0123
1,1,2-trimethylcyclohexane	0.0035
1,2,3-trimethylcyclohexane	0.0022
cis-1-ethyl-3-methylcyclohexane	0.0015
cis-1-ethyl-4-methylcyclohexane	0.0100
cis, cis-1,2,4-trimethylcyclohexane	0.0055
nonane	0.0256
trans-1-ethyl-2-methylcyclohexane	0.0022
cis, trans-1,2,3-trimethylcyclohexane	0.0044
trans-1-ethyl-4-methylcyclohexane	0.0156
2,4-dimethyloctane	0.0037
OTHER C10	0.0012
3,4-dimethyloctane	0.0060
isopropylcyclohexane	0.0129
3,5-dimethyloctane	0.0069
2,5-dimethyloctane	0.0018
cis-1-ethyl-2-methylcyclohexane	0.0055
propylcyclohexane	0.0262
2,6-dimethyloctane	0.0240
3,3,5-trimethylheptane	0.0031
OTHER C10	0.0068
3,6-dimethyloctane	0.0066
1,1,2,3-tetramethylcyclohexane	0.0182
3-ethyl-2-methylheptane	0.0057
1,1,3,5-tetramethylcyclohexane	0.0040
1,2-dimethyl-3-ethylcyclohexane	0.0062
1-ethyl-3-methylbenzene	0.0039
1,1,2,3-tetramethylcyclohexane	0.0202
OTHER C10	0.0040
4-ethyloctane	0.0087
4-methylnonane	0.0214
2-methylnonane	0.0382
3-methylnonane	0.0091
1-ethyl-2-methylbenzene	0.0202
OTHER C10	0.0015
1-methyl-4-isopropylcyclohexane	0.0033
1-methyl-3-isopropylcyclohexane	0.0145
1-methyl-3-isopropylcyclohexane	0.0093
1-ethyl-2,4-dimethylcyclohexane	0.0079
OTHER C10	0.0051
1,2,4-trimethylbenzene	0.0280
1-methyl-2-isopropylcyclohexane	0.0162
1-methyl-2-isopropylcyclohexane	0.0068
diethylcyclohexane	0.0052
decane	0.1008
methyl propylcyclohexane	0.0059
methyl propylcyclohexane	0.0090
methyl propylcyclohexane	0.0082
methyl propylcyclohexane	0.0033
diethylcyclohexane	0.0030
diethylcyclohexane	0.0016
2,4-dimethylnonane	0.0128
3,5-dimethylnonane	0.0074
2,5-dimethylnonane	0.0119
2,6-dimethylnonane	0.0274
methyl propylcyclohexane	0.0029
2,7-dimethylnonane	0.0128
isobutylcyclohexane	0.0088
butylcyclohexane	0.0078
pentylcyclopentane	0.0186
3,7-dimethylnonane	0.0091
4,5-dimethylnonane	0.0036
methyl propylcyclohexane	0.0083
4-ethylnonane	0.0082
5-methyldecane	0.0053
4-methyldecane	0.0171
2-methyldecane	0.0091
5-isopropylnonane	0.0108
3-methyldecane	0.0130
trans-decalin	0.0120
1,1-dimethyl-2-propylcyclohexane	0.0029
OTHER C11	0.0025
ethyl propylcyclohexane	0.0033
ethyl propylcyclohexane	0.0058
ethyl propylcyclohexane	0.0028
ethyl propylcyclohexane	0.0089
cis-decalin	0.0034
ethyl propylcyclohexane	0.0016
undecane	0.0446
1-ethyl-4-isopropylbenzene	0.0028
2-methyldecalin	0.0052
OTHER C12	0.0038
1,2,4,5-tetramethylbenzene	0.0027
1,2,3,5-tetramethylbenzene	0.0070
2,6-dimethyldecane	0.0024
2-methyldecalin	0.0018
3,7-dimethyldecane	0.0073
4,5-dimethyldecane	0.0013
(2-methylbutyl)cyclohexane	0.0023
pentylcyclohexane	0.0046
OTHER C12	0.0041
5-methylundecane	0.0050
4-methylundecane	0.0027
2-methylundecane	0.0036
3-methylundecane	0.0032
naphthalene	0.0014
dodecane	0.0105
2,6-dimethylundecane	0.0018
Total	1.0000
Fraction Identified	0.9710

SD24	
Compound	Fraction
methyl ethyl ketone	0.0010
4-methylheptane	0.0010
3-methylheptane	0.0030
octane	0.0011
cis-1,2-dimethylcyclohexane	0.0007
cis, cis-1,3,5-trimethylcyclohexane	0.0013
ethylcyclohexane	0.0006
1,1,3-trimethylcyclohexane	0.0016
ethylbenzene	0.0087
trans, trans-1,2,4-trimethylcyclohexane	0.0047
trans, trans-1,3,5-trimethylcyclohexane	0.0015
m-xylene	0.0288
p-xylene	0.0109
4-methyloctane	0.0025
2-methyloctane	0.0025
3-methyloctane	0.0005
1,2,3-trimethylcyclohexane	0.0052
o-xylene	0.0244
cis, trans-1,2,4-trimethylcyclohexane	0.0051
trans-1-ethyl-3-methylcyclohexane	0.0011
cis-1-ethyl-3-methylcyclohexane	0.0064
cis, cis-1,2,4-trimethylcyclohexane	0.0037
OTHER C9	0.0014
nonane	0.0162
1,2,3-trimethylcyclohexane	0.0021
cis, trans-1,2,3-trimethylcyclohexane	0.0033
trans-1-ethyl-4-methylcyclohexane	0.0104
cis-1-ethyl-4-methylcyclohexane	0.0023
isopropylbenzene	0.0031
2,3,5-trimethylheptane	0.0039
isopropylcyclohexane	0.0096
2,5-dimethyloctane	0.0046
3,5-dimethyloctane	0.0011
trans-bicyclo[4.3.0]nonane	0.0039
propylcyclohexane	0.0174
2,6-dimethyloctane	0.0156
3,3-dimethyloctane	0.0022
3,3,5-trimethylheptane	0.0048
3,6-dimethyloctane	0.0044
1-ethyl-2,4-dimethylcyclohexane	0.0121
3-ethyl-2-methylheptane	0.0140
propylbenzene	0.0021
3,3,4-trimethylheptane	0.0041
1-ethyl-3-methylbenzene	0.0394
1-ethyl-4-methylbenzene	0.0284
1,3,5-trimethylbenzene	0.0026
2,3-dimethyloctane	0.0381
4-methylnonane	0.0157
2-methylnonane	0.0122
1-ethyl-1,3-dimethylcyclohexane	0.0068
1-ethyl-2-methylbenzene	0.0138
3-ethyloctane	0.0143
3-methylnonane	0.0028
1-methyl-3-isopropylcyclohexane	0.0106
1-methyl-4-isopropylcyclohexane	0.0076
1-methyl-3-isopropylcyclohexane	0.0061
1,2-dimethyl-3-ethylcyclohexane	0.0038
1,2,4-trimethylbenzene	0.0763
1-methyl-2-isopropylcyclohexane	0.0125
1-methyl-2-isopropylcyclohexane	0.0051
2-ethyl-1,3-dimethylcyclohexane	0.0043
decane	0.0720
methyl propylcyclohexane	0.0043
methyl propylcyclohexane	0.0078
methyl propylcyclohexane	0.0073
methyl propylcyclohexane	0.0023
1,2,3,4-tetramethylcyclohexane	0.0021
1-methyl-3-isopropylbenzene	0.0017
diethylcyclohexane	0.0055
diethylcyclohexane	0.0040
1,2,3-trimethylbenzene	0.0166
2,5-dimethylnonane	0.0094
2,6-dimethylnonane	0.0205
2,4,6-trimethyloctane	0.0024
indane	0.0132
methyl propylcyclohexane	0.0065
sec butylcyclopentane	0.0063
butylcyclohexane	0.0145
pentylcyclopentane	0.0071
1-methyl-3-propylbenzene	0.0043
1-methyl-4-propylbenzene	0.0094
butylbenzene	0.0113
5-ethyl-2-methyloctane	0.0041
5-methyldecane	0.0148
4-methyldecane	0.0074
trans-decalin	0.0098
2-methyldecane	0.0015
5-isopropylnonane	0.0108
3-methyldecane	0.0116
1,4-dimethyl-2-ethylbenzene	0.0026
ethyl propylcyclohexane	0.0027
ethyl propylcyclohexane	0.0021
1,3-dimethyl-2-ethylbenzene	0.0044
1,3-dimethyl-2-ethylbenzene	0.0048
ethyl propylcyclohexane	0.0026
methyl butylcyclohexane	0.0086
methyl butylcyclohexane	0.0031
ethyl propylcyclohexane	0.0016
undecane	0.0405
1,2-dimethyl-3-ethylbenzene	0.0029
1-ethyl-4-isopropylbenzene	0.0050
cis-decalin	0.0038
3-phenylpentane	0.0028
1,2,4,5-tetramethylbenzene	0.0030
1,2,3,5-tetramethylbenzene	0.0070
2,6-dimethyldecane	0.0024
2-methyldecalin	0.0016
6-ethyl-2-methylnonane	0.0079
1-ethyl-3-isopropylbenzene	0.0012
5-methylindane	0.0025
1-ethyl-2-propylbenzene	0.0044
pentylcyclohexane	0.0049
1-ethyl-4-propylbenzene	0.0012
6-methylundecane	0.0051
4-methylundecane	0.0025
2-methylundecane	0.0037
3-methylundecane	0.0034
naphthalene	0.0016
methyl pentylcyclohexane	0.0007
1,3-dimethyl-5-isopropylbenzene	0.0013
dodecane	0.0111
1,1,5-trimethylindane	0.0010
2,6-dimethylundecane	0.0020
hexylcyclohexane	0.0006
Total	1.0000
Fraction Identified	0.9986

SD25	
Compound	Fraction
toluene	0.0027
4-methylheptane	0.0006
3-methylheptane	0.0016
octane	0.0009
cis-1,2-dimethylcyclohexane	0.0006
cis, cis-1,3,5-trimethylcyclohexane	0.0019
ethylcyclohexane	0.0006
1,1,3-trimethylcyclohexane	0.0021
ethylbenzene	0.0078
trans, trans-1,2,4-trimethylcyclohexane	0.0068
trans, trans-1,3,5-trimethylcyclohexane	0.0021
m-xylene	0.0208
p-xylene	0.0077
4-methyloctane	0.0027
3-methyloctane	0.0029
1,2,3-trimethylcyclohexane	0.0009
trans, cis-1,2,4-trimethylcyclohexane	0.0077
o-xylene	0.0143
cis, trans-1,2,4-trimethylcyclohexane	0.0034
cis, trans-1,2,4-trimethylcyclohexane	0.0021
trans-1-ethyl-3-methylcyclohexane	0.0015
cis-1-ethyl-3-methylcyclohexane	0.0090
OTHER C9	0.0051
OTHER C9	0.0018
nonane	0.0193
OTHER C10	0.0028
cis, trans-1,2,3-trimethylcyclohexane	0.0048
trans-1-ethyl-4-methylcyclohexane	0.0146
cis-1-ethyl-4-methylcyclohexane	0.0034
OTHER C10	0.0009
isopropylbenzene	0.0022
2,4-dimethyloctane	0.0053
2,3,5-trimethylheptane	0.0133
isopropylcyclohexane	0.0062
3,5-dimethyloctane	0.0015
2,5-dimethyloctane	0.0054
propylcyclohexane	0.0243
2,6-dimethyloctane	0.0209
3,3-dimethyloctane	0.0029
3,3,5-trimethylheptane	0.0064
3,6-dimethyloctane	0.0059
3-ethyl-2-methylheptane	0.0159
propylbenzene	0.0097
3,3,4-trimethylheptane	0.0033
1-ethyl-1,3-dimethylcyclohexane	0.0056
1-ethyl-3-methylbenzene	0.0187
1-ethyl-4-methylbenzene	0.0237
1,3,5-trimethylbenzene	0.0043
5-methylnonane	0.0322
4-methylnonane	0.0356
2-methylnonane	0.0088
1-ethyl-2-methylbenzene	0.0232
3-methylnonane	0.0035
1methyl-4-isopropylcyclohexane	0.0134
1-methyl-3-isopropylcyclohexane	0.0095
1-methyl-3-isopropylcyclohexane	0.0079
1,2-dimethyl-3-ethylcyclohexane	0.0047
1,2,4-trimethylbenzene	0.0402
1-methyl-2-isopropylcyclohexane	0.0166
1-methyl-2-isopropylcyclohexane	0.0118
decane	0.0832
methyl propylcyclohexane	0.0054
methyl propylcyclohexane	0.0084
methyl propylcyclohexane	0.0078
methyl propylcyclohexane	0.0029
1,2,3,4-tetramethylcyclohexane	0.0026
diethylcyclohexane	0.0020
1-methyl-3-isopropylbenzene	0.0105
1,2,3-trimethylbenzene	0.0113
2,5-dimethylnonane	0.0109
2,6-dimethylnonane	0.0227
2,4,6-trimethyloctane	0.0028
indane	0.0117
methyl propylcyclohexane	0.0085
isobutylcyclohexane	0.0070
butylcyclohexane	0.0169
1-methyl-3-propylbenzene	0.0078
1,3-diethylbenzene	0.0034
diethylcyclohexane	0.0082
1-methyl-4-propylbenzene	0.0086
5-ethyl-2-methyloctane	0.0049
5-methyldecane	0.0154
4-methyldecane	0.0077
trans-decalin	0.0089
2-methyldecane	0.0018
5-isopropylnonane	0.0127
3-methyldecane	0.0111
1,2-dimethyl-4-ethylbenzene	0.0031
1,3-dimethyl-2-ethylbenzene	0.0024
1-methylindane	0.0034
ethyl propylcyclohexane	0.0061
1,4-dimethyl-2-ethylbenzene	0.0026
OTHER C11	0.0104
1,2,3-trimethyl-4-ethylbenzene	0.0022
2-phenylpentane	0.0019
undecane	0.0378
1-ethyl-4-isopropylbenzene	0.0080
diethylcyclohexane	0.0041
ethyl propylcyclohexane	0.0029
1,2,4,5-tetramethylbenzene	0.0029
1,2,3,5-tetramethylbenzene	0.0067
2,6-dimethyldecane	0.0026
2-methyldecalin	0.0015
4,5-dimethyldecane	0.0088
1-ethyl-3-isopropylbenzene	0.0012
5-methylindane	0.0025
pentylcyclohexane	0.0047
4-methylindane	0.0057
1-ethyl-4-propylbenzene	0.0012
6-methylundecane	0.0053
5-methylundecane	0.0027
2-methylundecane	0.0049
3-methylundecane	0.0037
naphthalene	0.0016
methyl pentylcyclohexane	0.0010
5,6-dimethylindane	0.0016
dodecane	0.0123
2,5-dimethylundecane	0.0007
OTHER C13	0.0025
Total	1.0000
Fraction Identified	0.9938

SD26	
Compound	Fraction
acetone	0.0024
2-propanol	0.0014
OTHER C7	0.0007
toluene	0.0007
OTHER C8	0.0008
1,1,2-trimethylcyclopentane	0.0019
2-methylheptane	0.0005
cis-1,3-dimethylcyclohexane	0.0006
octane	0.0029
cis, cis-1,3,5-trimethylcyclohexane	0.0008
ethylcyclohexane	0.0011
1,1,3-trimethylcyclohexane	0.0007
OTHER C9	0.0005
OTHER C9	0.0009
ethylbenzene	0.0105
2,6-dimethylheptane	0.0043
trans, trans-1,2,4-trimethylcyclohexane	0.0011
m-xylene	0.0215
p-xylene	0.0076
OTHER C9	0.0021
OTHER C9	0.0017
cis-1-ethyl-2-methylcyclohexane	0.0047
o-xylene	0.0132
1,1,2-trimethylcyclohexane	0.0030
OTHER C9	0.0006
cis-1-ethyl-3-methylcyclohexane	0.0064
cis, cis-1,2,4-trimethylcyclohexane	0.0035
nonane	0.0116
trans-1-ethyl-2-methylcyclohexane	0.0012
trans-1-ethyl-2-methylcyclohexane	0.0029
1-ethyl-1-methylcyclohexane	0.0101
OTHER C10	0.0022
isopropylbenzene	0.0035
2,4-dimethyloctane	0.0039
2,5-dimethyloctane	0.0069
isopropylcyclohexane	0.0047
OTHER C10	0.0011
OTHER C10	0.0040
2,6-dimethyloctane	0.0169
propylcyclohexane	0.0159
3,3-dimethyloctane	0.0018
3,6-dimethyloctane	0.0041
3-ethyl-2-methylheptane	0.0043
1,1,2,3-tetramethylcyclohexane	0.0116
propylbenzene	0.0193
4-ethyloctane	0.0034
1-ethyl-3-methylbenzene	0.0524
1-ethyl-4-methylbenzene	0.0346
1,3,5-trimethylbenzene	0.0491
2-methylnonane	0.0271
3-ethyloctane	0.0066
3-methylnonane	0.0341
1-methyl-2-ethylbenzene	0.0018
1,1,2,3-tetramethylcyclohexane	0.0099
1-methyl-3-isopropylcyclohexane	0.0057
1-methyl-3-isopropylcyclohexane	0.0058
1,1,3,4-tetramethylcyclohexane	0.0030
1,2,4-trimethylbenzene	0.0979
diethylcyclohexane	0.0114
diethylcyclohexane	0.0079
decane	0.0732
sec-butylbenzene	0.0036
diethylcyclohexane	0.0071
1-methyl-3-isopropylbenzene	0.0087
2,4-dimethylnonane	0.0028
methyl propylcyclohexane	0.0061
1,2,3-trimethylbenzene	0.0215
diethylcyclohexane	0.0077
2,6-dimethylnonane	0.0182
butylcyclohexane	0.0018
1-methyl-2-isopropylbenzene	0.0131
3,6-dimethylnonane	0.0049
4,5-dimethylnonane	0.0054
3,7-dimethylnonane	0.0128
methyl propylcyclohexane	0.0064
1,3-diethylbenzene	0.0044
4-ethylnonane	0.0098
1,3-dimethyl-5-ethylbenzene	0.0121
5-methyldecane	0.0032
4-methyldecane	0.0128
2-methyldecane	0.0072
trans-decalin	0.0095
OTHER C11	0.0013
3-methyldecane	0.0097
1,4-dimethyl-2-ethylbenzene	0.0105
1,3-dimethyl-4-ethylbenzene	0.0022
ethyl propylcyclohexane	0.0022
ethyl propylcyclohexane	0.0016
1,3-dimethyl-2-ethylbenzene	0.0039
ethyl propylcyclohexane	0.0035
ethyl propylcyclohexane	0.0018
cis-decalin	0.0073
OTHER C11	0.0026
OTHER C11	0.0016
dodecane	0.0435
1-ethyl-4-isopropylbenzene	0.0024
2-methyldecalin	0.0043
4,6-dimethyldecane	0.0061
(2-methylbutyl)benzene	0.0026
1,2,3,5-tetramethylbenzene	0.0067
2-methyldecalin	0.0022
2,6-dimethyldecane	0.0019
3,7-dimethyldecane	0.0073
OTHER C12	0.0013
OTHER C12	0.0009
OTHER C12	0.0010
(2-methylbutyl)cyclohexane	0.0049
OTHER C12	0.0041
4-ethyldecane	0.0011
6-methylundecane	0.0030
5-methylundecane	0.0023
4-methylundecane	0.0033
1,2,3,4-tetramethylbenzene	0.0041
2-methylundecane	0.0007
3-methylundecane	0.0037
naphthalene	0.0008
methyl pentylcyclohexane	0.0012
dodecane	0.0147
2,4-dimethylundecane	0.0006
2,5-dimethylundecane	0.0016
Total	1.0000
Fraction Identified	0.9725

SD27	
Compound	Fraction
2-methylheptane	0.0007
4-methylheptane	0.0017
3-ethylhexane	0.0005
octane	0.0011
ethylcyclohexane	0.0012
1,1,3-trimethylcyclohexane	0.0012
ethylbenzene	0.0019
trans, trans-1,3,5-trimethylcyclohexane	0.0061
OTHER C9	0.0016
m-xylene	0.0049
p-xylene	0.0019
4-methyloctane	0.0024
3-methyloctane	0.0027
1,2,3-trimethylcyclohexane	0.0076
o-xylene	0.0068
cis, trans-1,2,4-trimethylcyclohexane	0.0067
1,1,2-trimethylcyclohexane	0.0021
cis-1-ethyl-3-methylcyclohexane	0.0109
trans-1-ethyl-3-methylcyclohexane	0.0061
cis, cis-1,2,4-trimethylcyclohexane	0.0013
OTHER C9	0.0008
nonane	0.0285
trans-1-ethyl-2-methylcyclohexane	0.0031
cis, trans-1,2,3-trimethylcyclohexane	0.0052
trans-1-ethyl-4-methylcyclohexane	0.0168
cis-1-ethyl-4-methylcyclohexane	0.0039
isopropylbenzene	0.0011
2,4,6-trimethylheptane	0.0059
3,5-dimethyloctane	0.0151
2,5-dimethyloctane	0.0069
3,5-dimethyloctane	0.0017
2,7-dimethyloctane	0.0059
propylcyclohexane	0.0272
2,6-dimethyloctane	0.0267
2,2,3,3-tetramethylhexane	0.0031
OTHER C10	0.0068
3,6-dimethyloctane	0.0067
diethylcyclohexane	0.0177
propylbenzene	0.0055
OTHER C10	0.0040
2,3-dimethyloctane	0.0063
1-ethyl-3-methylbenzene	0.0040
1-ethyl-4-methylbenzene	0.0187
3-ethyl-4-methylheptane	0.0053
5-methylnonane	0.0083
1,3,5-trimethylbenzene	0.0207
4-methylnonane	0.0422
3-ethyloctane	0.0097
3-methylnonane	0.0192
trans-decalin	0.0054
diethylcyclohexane	0.0155
1-methyl-3-isopropylcyclohexane	0.0107
1,2-dimethyl-3-ethylcyclohexane	0.0096
1,2-dimethyl-3-ethylcyclohexane	0.0059
1,2,4-trimethylbenzene	0.0278
1-methyl-2-isopropylcyclohexane	0.0185
cis-decalin	0.0071
methyl butylcyclopentane	0.0070
decane	0.0923
methyl propylcyclohexane	0.0060
methyl propylcyclohexane	0.0093
diethylcyclohexane	0.0086
methyl propylcyclohexane	0.0036
OTHER C11	0.0030
methyl propylcyclohexane	0.0024
1,2,3-trimethylbenzene	0.0136
2,4-dimethylnonane	0.0076
2,5-dimethylnonane	0.0071
OTHER C11	0.0056
2,6-dimethylnonane	0.0281
methyl propylcyclohexane	0.0035
isobutylcyclohexane	0.0137
pentylcyclopentane	0.0094
OTHER C11	0.0087
butylcyclohexane	0.0166
3,7-dimethylnonane	0.0122
methyl propylcyclohexane	0.0034
5-methylindane	0.0089
1,3-dimethyl-5-ethylbenzene	0.0079
5-ethyl-2-methyloctane	0.0060
5-methyldecane	0.0192
4-methyldecane	0.0096
2-methyldecane	0.0106
5-isopropylnonane	0.0020
2,3-dimethylnonane	0.0133
1,4-dimethyl-2-ethylbenzene	0.0140
1,3-dimethyl-4-ethylbenzene	0.0036
OTHER C11	0.0026
1,3-dimethyl-2-ethylbenzene	0.0030
diethylcyclohexane	0.0053
ethyl propylcyclohexane	0.0027
ethyl propylcyclohexane	0.0104
cis-decalin	0.0024
1-ethyl-2-isopropylcyclohexane	0.0017
undecane	0.0341
2-methyldecalin	0.0081
4,6-dimethyldecane	0.0041
(2-methylbutyl)benzene	0.0030
1,2,3,5-tetramethylbenzene	0.0073
2,6-dimethyldecane	0.0023
2-methyldecalin	0.0022
3,7-dimethyldecane	0.0088
1-methyl-3-butylbenzene	0.0015
(2-methylbutyl)cyclohexane	0.0024
pentylcyclohexane	0.0042
4-ethyldecane	0.0050
OTHER C12	0.0012
tetralin	0.0053
4-methylundecane	0.0025
2-methylundecane	0.0044
3-methylundecane	0.0034
naphthalene	0.0014
2-butyl-1,3-dimethylcyclohexane	0.0009
5,6-dimethylindane	0.0013
dodecane	0.0108
OTHER C13	0.0007
2,6-dimethylundecane	0.0025
5-methyldodecane	0.0006
Total	1.0000
Fraction Identified	0.9718

SD28	
Compound	fraction
acetone	0.0029
2-propanol	0.0014
tert-butyl alcohol	0.0028
methyl ethyl ketone	0.0116
methyl propyl ketone	0.1454
trans-1,3-dimethylcyclopentane	0.0007
heptane	0.0058
methyl isobutyl ketone	0.0067
methylcyclohexane	0.0157
1,1,3-trimethylcyclopentane	0.0017
2,5-dimethylhexane	0.0010
2,4-dimethylhexane	0.0024
1,2,4-trimethylcyclopentane	0.0036
1,2,3-trimethylcyclopentane	0.0036
toluene	0.0536
2,3-dimethylhexane	0.0024
3-ethyl-2-methylpentane	0.0007
1,1,2-trimethylcyclopentane	0.0014
2-methylheptane	0.0215
4-methylheptane	0.0058
3,4-dimethylhexane	0.0018
3-methylheptane	0.0140
3-ethylhexane	0.0030
3,3-dimethylhexane	0.0009
cis-1,3-dimethylcyclohexane	0.0308
trans-1,4-dimethylcyclohexane	0.0118
1,1-dimethylcyclohexane	0.0035
cis-1-ethyl-3-methylcyclopentane	0.0020
trans-1-ethyl-3-methylcyclopentane	0.0019
cis-1-ethyl-2-methylcyclopentane	0.0039
trans-1,2-dimethylcyclohexane	0.0012
octane	0.0606
cis-1,4-dimethylcyclohexane	0.0023
trans-1,3-dimethylcyclohexane	0.0130
OTHER C9	0.0015
OTHER C9	0.0008
2,2-dimethylheptane	0.0023
2,4-dimethylheptane	0.0034
2,6-dimethylheptane	0.0113
propylcyclopentane	0.0015
cis, cis-1,3,5-trimethylcyclohexane	0.0099
ethylcyclohexane	0.0165
2,5-dimethylheptane	0.0049
1,1,3-trimethylcyclohexane	0.0109
1,1,4-trimethylcyclohexane	0.0028
OTHER C9	0.0014
ethylbenzene	0.0141
trans, trans-1,2,4-trimethylcyclohexane	0.0199
trans, trans-1,3,5-trimethylcyclohexane	0.0049
OTHER C9	0.0036
m-xylene	0.0343
p-xylene	0.0106
4-methyloctane	0.0047
methyl amyl ketone	0.0055
2-methyloctane	0.0014
bicyclo[3.3.0]octane	0.0014
3-methyloctane	0.0023
trans, cis-1,2,4-trimethylcyclohexane	0.0104
o-xylene	0.0185
cis, trans-1,2,4-trimethylcyclohexane	0.0054
cis-1-ethyl-3-methylcyclohexane	0.0065
trans-1-ethyl-3-methylcyclohexane	0.0028
nonane	0.0049
cis, trans-1,2,3-trimethylcyclohexane	0.0021
trans-1-ethyl-2-methylcyclohexane	0.0057
cis-1-ethyl-4-methylcyclohexane	0.0012
2,3,5-trimethylheptane	0.0022
OTHER C10	0.0009
bicyclo[3.3.0]octane	0.0028
2,5-dimethyloctane	0.0022
3,5-dimethyloctane	0.0019
propylcyclohexane	0.0081
2,6-dimethyloctane	0.0075
3,3,5-trimethylheptane	0.0034
OTHER C10	0.0022
1,2-dimethyl-3-ethylcyclohexane	0.0060
1,1,2,3-tetramethylcyclohexane	0.0024
OTHER C10	0.0014
OTHER C10	0.0021
1-ethyl-3-methylbenzene	0.0044
1-ethyl-4-methylbenzene	0.0098
5-methylnonane	0.0043
4-methylnonane	0.0093
2,3-dimethyloctane	0.0081
2-methylnonane	0.0059
OTHER C10	0.0035
1-ethyl-2-methylbenzene	0.0091
3-methylnonane	0.0010
1-methyl-3-isopropylcyclohexane	0.0053
1-methyl-3-isopropylcyclohexane	0.0033
3-methylstyrene	0.0195
1,2,4-trimethylbenzene	0.0047
4-methylstyrene	0.0189
bicyclo[3.3.1]nonane	0.0063
1-methyl-2-isopropylcyclohexane	0.0043
decane	0.0384
sec butylbenzene	0.0023
methyl propylcyclohexane	0.0031
methyl propylcyclohexane	0.0031
OTHER C11	0.0010
1-methyl-3-isopropylbenzene	0.0045
1,2,3-trimethylbenzene	0.0036
2,5-dimethylnonane	0.0037
2,4,6-trimethyloctane	0.0095
indane	0.0053
methyl propylcyclohexane	0.0035
OTHER C11	0.0028
butylcyclohexane	0.0067
3,7-dimethylnonane	0.0034
methyl propylcyclohexane	0.0026
butylbenzene	0.0022
5-ethyl-2-methyloctane	0.0017
5-methyldecane	0.0038
4-methyldecane	0.0039
trans-decalin	0.0038
1,4-dimethyl-2-ethylbenzene	0.0056
3-methyldecane	0.0044
ethyl propylcyclohexane	0.0012
ethyl propylcyclohexane	0.0038
undecane	0.0199
1-ethyl-4-isopropylbenzene	0.0022
diethylcyclohexane	0.0018
3,5-dimethyldecane	0.0027
4,5-dimethyldecane	0.0031
pentylcyclohexane	0.0024
OTHER C12	0.0013
2,3-dimethyldecane	0.0021
4-methylundecane	0.0009
2-methylundecane	0.0015
3-methylundecane	0.0017
dodecane	0.0058
2,6-dimethylundecane	0.0012
Total	1.0000
Fraction Identified	0.9807

SD29	
Compound	Fraction
methyl ethyl ketone	0.0020
methyl isobutyl ketone	0.0016
methylcyclohexane	0.0006
2-methylheptane	0.0009
4-methylheptane	0.0007
3,4-dimethylhexane	0.0009
3-methylheptane	0.0011
cis-1,3-dimethylcyclohexane	0.0012
octane	0.0026
cis-1,2-dimethylcyclohexane	0.0013
cis, cis-1,3,5-trimethylcyclohexane	0.0011
ethylcyclohexane	0.0013
1,1,3-trimethylcyclohexane	0.0025
ethylbenzene	0.0059
trans, trans-1,2,4-trimethylcyclohexane	0.0058
trans, trans-1,3,5-trimethylcyclohexane	0.0010
m-xylene	0.0166
p-xylene	0.0061
4-methyloctane	0.0031
3-methyloctane	0.0027
trans, cis-1,2,4-trimethylcyclohexane	0.0062
o-xylene	0.0079
cis, trans-1,2,4-trimethylcyclohexane	0.0037
trans-1-ethyl-3-methylcyclohexane	0.0009
cis-1-ethyl-3-methylcyclohexane	0.0070
trans-1-ethyl-4-methylcyclohexane	0.0037
nonane	0.0120
1,2,3-trimethylcyclohexane	0.0012
cis, trans-1,2,3-trimethylcyclohexane	0.0038
trans-1-ethyl-2-methylcyclohexane	0.0114
cis-1-ethyl-4-methylcyclohexane	0.0025
isopropylbenzene	0.0014
2,4,5-trimethylheptane	0.0047
3,4-dimethyloctane	0.0022
isopropylcyclohexane	0.0066
2,5-dimethyloctane	0.0055
3,5-dimethyloctane	0.0013
2,7-dimethyloctane	0.0051
propylcyclohexane	0.0211
2,6-dimethyloctane	0.0200
3,3,5-trimethylheptane	0.0096
3,6-dimethyloctane	0.0063
1,2-dimethyl-3-ethylcyclohexane	0.0164
3-ethyl-2-methylheptane	0.0051
propylbenzene	0.0035
3,3,4-trimethylheptane	0.0048
1-ethyl-3-methylbenzene	0.0064
1-ethyl-4-methylbenzene	0.0207
1,3,5-trimethylbenzene	0.0121
5-methylnonane	0.0237
4-methylnonane	0.0208
2-methylnonane	0.0173
1-ethyl-1,3-dimethylcyclohexane	0.0094
3-methylnonane	0.0210
1-ethyl-2-methylbenzene	0.0012
1-methyl-4-isopropylcyclohexane	0.0028
1-methyl-3-isopropylcyclohexane	0.0135
1-methyl-3-isopropylcyclohexane	0.0090
1-methyl-4-isopropylcyclohexane	0.0084
diethylcyclohexane	0.0049
1,2,4-trimethylbenzene	0.0343
1-methyl-2-isopropylcyclohexane	0.0176
1-methyl-2-isopropylcyclohexane	0.0116
decane	0.0980
diethylcyclohexane	0.0061
methyl propylcyclohexane	0.0091
diethylcyclohexane	0.0083
diethylcyclohexane	0.0033
1,2,3,4-tetramethylcyclohexane	0.0028
1,2,3-trimethylbenzene	0.0138
sec butylcyclohexane	0.0090
2,5-dimethylnonane	0.0110
2,4,6-trimethyloctane	0.0327
methyl propylcyclohexane	0.0156
methyl propylcyclohexane	0.0083
isobutylcyclohexane	0.0084
butylcyclohexane	0.0195
pentylcyclopentane	0.0109
3,6-dimethylnonane	0.0034
3,7-dimethylnonane	0.0080
4-ethylnonane	0.0069
1-ethyl-2,2,6-trimethylcyclohexane	0.0057
3-ethylnonane	0.0033
5-methyldecane	0.0123
2-methyldecane	0.0132
trans-decalin	0.0123
5-isopropylnonane	0.0041
ethyl propylcyclohexane	0.0112
3-methyldecane	0.0138
ethyl propylcyclohexane	0.0031
ethyl propylcyclohexane	0.0035
ethyl propylcyclohexane	0.0024
diethylcyclohexane	0.0044
methyl butylcyclohexane	0.0027
cis-decalinis	0.0123
methyl butylcyclohexane	0.0022
undecane	0.0611
2-methyldecalin	0.0090
2,4-dimethyldecane	0.0060
OTHER C12	0.0019
2,6-dimethyldecane	0.0091
2-methyldecalin	0.0026
3,7-dimethyldecane	0.0024
4,5-dimethyldecane	0.0094
5-sec butylnonane	0.0015
OTHER C12	0.0023
pentylcyclohexane	0.0071
hexylcyclopentane	0.0044
4-ethyldecane	0.0014
6-methylundecane	0.0062
5-methylundecane	0.0032
2-methylundecane	0.0052
3-methylundecane	0.0039
dodecane	0.0126
2,6-dimethylundecane	0.0015
Total	1.0000
Fraction Identified	0.9929

SD30	
Compound	Fraction
methanol	0.0021
acetone	0.0185
2-propanol	0.0473
methyl ethyl ketone	0.0514
EtOAc	0.0034
isobutyl alcohol	0.0058
butyl alcohol	0.0047
2-methylhexane	0.0007
3-methylhexane	0.0011
cis-1,3-dimethylcyclopentane	0.0006
1,2-dimethylcyclopentane	0.0008
heptane	0.0037
methyl isobutyl ketone	0.0010
methylcyclohexane	0.0060
2,4-dimethylhexane	0.0007
1,2,4-trimethylcyclopentane	0.0006
1,2,3-trimethylcyclopentane	0.0006
toluene	0.0400
4-methylheptane	0.0028
2,3-dimethylhexane	0.0007
3-methylheptane	0.0015
cis-1,3-dimethylcyclohexane	0.0030
trans-1,4-dimethylcyclohexane	0.0010
butyl acetate	0.0176
octane	0.0047
trans-1,3-dimethylcyclohexane	0.0011
2,6-dimethylheptane	0.0009
ethylcyclohexane	0.0012
methyl isoamyl ketone	0.0013
1,1,3-trimethylcyclohexane	0.0008
ethylbenzene	0.0118
trans, trans-1,2,4-trimethylcyclohexane	0.0013
m-xylene	0.0326
p-xylene	0.0117
methyl amyl ketone	0.6876
o-xylene	0.0162
2-butoxyethanol	0.0063
nonane	0.0007
1-ethyl-3-methylbenzene	0.0006
1-ethyl-4-methylbenzene	0.0008
1,3,5-trimethylbenzene	0.0008
1,2,4-trimethylbenzene	0.0012
decane	0.0015
undecane	0.0006
dodecane	0.0009
Total	1.0000
Fraction Identified	1.0000

SD31	
Compound	Fraction
ethanol	0.0072
isobutyl alcohol	0.0116
butyl alcohol	0.0059
methyl propyl ketone	0.0773
methyl isobutyl ketone	0.0046
toluene	0.1138
butyl acetate	0.6121
ethylbenzene	0.0102
m-xylene	0.0296
p-xylene	0.0110
o-xylene	0.0142
nonane	0.0020
ethyl-3-ethoxypropionate	0.0033
decane	0.0038
acetophenone	0.0128
2-phenyl-2-propanol	0.0080
diethyl fumarate	0.0674
dodecane	0.0032
tridecane	0.0021
Total	1.0000
Fraction Identified	1.0000

SD32	
Compound	Fraction
2-propanol	0.0042
methyl ethyl ketone	0.0120
isobutyl alcohol	0.0018
1,1-dimethylcyclopentane	0.0012
2-methylhexane	0.0008
cis-1,3-dimethylcyclopentane	0.0009
heptane	0.0074
methylcyclohexane	0.0165
1,1,3-trimethylcyclopentane	0.0013
2,5-dimethylhexane	0.0008
2,4-dimethylhexane	0.0017
1,2,4-trimethylcyclopentane	0.0015
1,2,3-trimethylcyclopentane	0.0011
toluene	0.0209
2-methylheptane	0.0045
4-methylheptane	0.0026
3,4-dimethylhexane	0.0049
3-methylheptane	0.0023
cis-1,3-dimethylcyclohexane	0.0041
trans-1,4-dimethylcyclohexane	0.0014
butyl acetate	0.0772
octane	0.0063
cis-1,4-dimethylcyclohexane	0.0015
2,6-dimethylheptane	0.0013
Bz/Cl	0.0000
ethylcyclohexane	0.0017
1,1,3-trimethylcyclohexane	0.0013
ethylbenzene	0.0107
trans, trans-1,3,5-trimethylcyclohexane	0.0063
trans, trans-1,2,4-trimethylcyclohexane	0.0008
m-xylene	0.0334
p-xylene	0.0120
4-methyloctane	0.0018
3-methyloctane	0.0017
trans, cis-1,2,4-trimethylcyclohexane	0.0058
1,2,3-trimethylcyclohexane	0.0190
cis, trans-1,2,4-trimethylcyclohexane	0.0038
o-xylene	0.0063
cis, cis-1,2,4-trimethylcyclohexane	0.0030
nonane	0.0060
1,2,3-trimethylcyclohexane	0.0008
cis, trans-1,2,3-trimethylcyclohexane	0.0028
trans-1-ethyl-4-methylcyclohexane	0.0094
cis-1-ethyl-4-methylcyclohexane	0.0021
isopropylbenzene	0.0035
3,4-dimethyloctane	0.0014
2,4-dimethyloctane	0.0047
2,5-dimethyloctane	0.0043
3,5-dimethyloctane	0.0010
propylcyclohexane	0.0037
2,6-dimethyloctane	0.0166
3,3-dimethyloctane	0.0148
OTHER C10	0.0062
3-ethyl-2-methylheptane	0.0044
5-ethyl-2-methylheptane	0.0118
3,6-dimethyloctane	0.0043
3,3,4-trimethylheptane	0.0027
1-ethyl-3-methylbenzene	0.0038
1-ethyl-4-methylbenzene	0.0065
4-methylnonane	0.0124
ethyl-3-ethoxypropionate	0.1633
2,3-dimethyloctane	0.0054
2-methylnonane	0.0177
3-ethyloctane	0.0156
1-ethyl-2-methylbenzene	0.0105
3-methylnonane	0.0067
1,3-dimethyl-2-isopropylcyclopentane	0.0162
1-methyl-4-isopropylcyclohexane	0.0020
1,4-dimethyl-1-ethylcyclohexane	0.0099
1-methyl-3-isopropylcyclohexane	0.0062
1,2-dimethyl-3-ethylcyclohexane	0.0057
1,2,4-trimethylbenzene	0.0033
1-methyl-2-isopropylcyclohexane	0.0280
bicyclo[3.3.1]nonane	0.0119
1,2-dimethyl-3-ethylcyclohexane	0.0045
1-methyl-2-isopropylcyclohexane	0.0032
decane	0.0642
methyl propylcyclohexane	0.0045
methyl propylcyclohexane	0.0058
1,4-dimethyl-1-ethylcyclohexane	0.0056
diethylcyclohexane	0.0023
1-methyl-3-isopropylbenzene	0.0020
1,2,3-trimethylbenzene	0.0081
sec butylcyclohexane	0.0067
2,4,6-trimethyloctane	0.0063
2,6-dimethylnonane	0.0151
2,7-dimethylnonane	0.0096
methyl propylcyclohexane	0.0055
isobutylcyclohexane	0.0046
butylcyclohexane	0.0113
pentylcyclopentane	0.0057
3,7-dimethylnonane	0.0049
4-ethylnonane	0.0037
OTHER C11	0.0030
3-ethylnonane	0.0019
5-ethyl-2-methyloctane	0.0063
5-methyldecane	0.0063
4-methyldecane	0.0058
trans-decalin	0.0092
3-methyldecane	0.0068
OTHER C11	0.0017
OTHER C11	0.0011
ethyl propylcyclohexane	0.0035
cis-decalin	0.0054
undecane	0.0247
OTHER C12	0.0040
OTHER C12	0.0037
2,6-dimethyldecane	0.0041
2-methyldecalin	0.0014
6-ethyl-2-methylnonane	0.0043
pentylcyclohexane	0.0033
2,3-dimethyldecane	0.0018
6-methylundecane	0.0015
5-methylundecane	0.0011
4-methylundecane	0.0015
2-methylundecane	0.0022
3,8-dimethyldecane	0.0023
dodecane	0.0069
2,6-dimethylundecane	0.0009
Total	1.0000
Fraction Identified	0.9831

SD33	
Compound	Fraction
acetone	0.0014
2-propanol	0.0182
methyl ethyl ketone	0.1552
isobutyl alcohol	0.0025
2-methylhexane	0.0019
2,3-dimethylpentane	0.0008
3-methylhexane	0.0045
trans-1,3-dimethylcyclopentane	0.0022
cis-1,3-dimethylcyclopentane	0.0031
1,2-dimethylcyclopentane	0.0050
heptane	0.0384
methylcyclohexane	0.0838
1,1,3-trimethylcyclopentane	0.0063
2,5-dimethylhexane	0.0039
2,4-dimethylhexane	0.0086
1,2,4-trimethylcyclopentane	0.0074
1,2,3-trimethylcyclopentane	0.0056
2,3,4-trimethylpentane	0.0008
toluene	0.0935
2,3-dimethylhexane	0.0030
3-ethyl-2-methylpentane	0.0008
1,1,2-trimethylcyclopentane	0.0020
2-methylheptane	0.0197
4-methylheptane	0.0062
3,4-dimethylhexane	0.0013
3,4-dimethylhexane	0.0023
3-methylheptane	0.0118
3-ethylhexane	0.0030
cis-1,3-dimethylcyclohexane	0.0191
trans-1,4-dimethylcyclohexane	0.0069
1,1-dimethylcyclohexane	0.0021
cis-1-ethyl-3-methylcyclopentane	0.0009
cis-1-ethyl-2-methylcyclopentane	0.0008
butyl acetate	0.0026
trans-1,2-dimethylcyclohexane	0.0045
octane	0.0286
trans-1,3-dimethylcyclohexane	0.0007
cis-1,4-dimethylcyclohexane	0.0071
OTHER C9	0.0005
2,2,5-trimethylhexane	0.0012
2,4-dimethylheptane	0.0018
cis-1,2-dimethylcyclohexane	0.0062
Bz/Cl	0.0000
ethylcyclohexane	0.0081
2,5-dimethylheptane	0.0030
1,1,3-trimethylcyclohexane	0.0049
1,1,4-trimethylcyclohexane	0.0011
OTHER C9	0.0006
ethylbenzene	0.0075
trans, trans-1,2,4-trimethylcyclohexane	0.0098
trans, trans-1,3,5-trimethylcyclohexane	0.0042
m-xylene	0.0207
p-xylene	0.0083
4-methyloctane	0.0021
2-methyloctane	0.0030
cis-bicyclo[3.3.0]octane	0.0007
3-methyloctane	0.0030
trans, cis-1,2,4-trimethylcyclohexane	0.0064
o-xylene	0.0149
cis, trans-1,2,4-trimethylcyclohexane	0.0032
cis-1-ethyl-3-methylcyclohexane	0.0047
trans-1-ethyl-3-methylcyclohexane	0.0022
nonane	0.0048
cis, trans-1,2,3-trimethylcyclohexane	0.0018
trans-1-ethyl-4-methylcyclohexane	0.0052
cis-1-ethyl-4-methylcyclohexane	0.0011
isopropylbenzene	0.0013
2,3,5-trimethylheptane	0.0016
isopropylcyclohexane	0.0034
2,5-dimethyloctane	0.0019
3,5-dimethyloctane	0.0018
propylcyclohexane	0.0078
2,6-dimethyloctane	0.0068
3,3-dimethyloctane	0.0010
2,2,3,3-tetramethylhexane	0.0021
diethylcyclohexane	0.0020
3-ethyl-2-methylheptane	0.0055
propylbenzene	0.0036
OTHER C10	0.0011
4-methylnonane	0.0017
1-ethyl-3-methylbenzene	0.0104
1-ethyl-4-methylbenzene	0.0106
2,3-dimethyloctane	0.0171
1,3,5-trimethylbenzene	0.0073
3-ethyloctane	0.0066
2-methylnonane	0.0031
1-ethyl-2-methylbenzene	0.0102
3-methylnonane	0.0011
1-methyl-3-isopropylcyclohexane	0.0053
1-methyl-3-isopropylcyclohexane	0.0029
1-methyl-4-isopropylcyclohexane	0.0029
OTHER C10	0.0016
1,2,4-trimethylbenzene	0.0303
OTHER C10	0.0060
1,2-dimethyl-3-ethylcyclohexane	0.0039
decane	0.0317
methyl propylcyclohexane	0.0024
methyl propylcyclohexane	0.0029
methyl propylcyclohexane	0.0030
OTHER C11	0.0010
OTHER C11	0.0015
1,2,3-trimethylbenzene	0.0106
2,5-dimethylnonane	0.0035
2,7-dimethylnonane	0.0084
methyl propylcyclohexane	0.0047
methyl propylcyclohexane	0.0028
OTHER C11	0.0022
butylcyclohexane	0.0062
1-methyl-3-propylbenzene	0.0027
5-methylindane	0.0037
butylbenzene	0.0025
5-ethyl-2-methyloctane	0.0014
5-methyldecane	0.0044
4-methyldecane	0.0027
trans-decalin	0.0038
1,4-dimethyl-2-ethylbenzene	0.0048
3-methyldecane	0.0031
1,2-dimethyl-4-ethylbenzene	0.0008
1-methylindane	0.0009
1,3-dimethyl-2-ethylbenzene	0.0018
ethyl propylcyclohexane	0.0023
undecane	0.0119
ethyl propylcyclohexane	0.0007
1-ethyl-4-isopropylbenzene	0.0013
2,5-dimethyldecane	0.0016
2-methyldecalin	0.0018
OTHER C12	0.0011
4-methylindane	0.0008
6-methylundecane	0.0012
4-methylundecane	0.0005
2-methylundecane	0.0009
3-methylundecane	0.0007
dodecane	0.0035
Total	1.0000
Fraction Identified	0.9860

SD34	
Compound	Fraction
ethanol	0.0028
butyl alcohol	0.0307
toluene	0.0013
2-propoxyethanol	0.2919
butyl acetate	0.0031
Bz/Cl	0.0000
ethylbenzene	0.0148
m-xylene	0.0377
p-xylene	0.0139
methyl amyl ketone	0.0574
o-xylene	0.0106
1-ethyl-3-methylbenzene	0.0029
1-ethyl-4-methylbenzene	0.0014
ethyl-3-ethoxypropionate	0.0137
1,3,5-trimethylbenzene	0.0033
1-ethyl-2-methylbenzene	0.0024
1,2,4-trimethylbenzene	0.0254
1-methyl-3-isopropylbenzene	0.0012
1,2,3-trimethylbenzene	0.0183
indane	0.0063
1,3-diethylbenzene	0.0086
1-methyl-3-propylbenzene	0.0233
1,4-diethylbenzene	0.0202
1-methyl-4-propylbenzene	0.0355
1,2-diethylbenzene	0.0018
1-methyl-2-propylbenzene	0.0108
1,4-dimethyl-2-ethylbenzene	0.0263
1,3-dimethyl-4-ethylbenzene	0.0271
1,3-dimethyl-2-ethylbenzene	0.0524
1-methylindane	0.0019
1,3-dimethyl-2-ethylbenzene	0.0029
2-phenylpentane	0.0034
1-ethyl-4-isopropylbenzene	0.0018
1,2-dimethyl-3-ethylbenzene	0.0119
3-phenylpentane	0.0016
1,2,4,5-tetramethylbenzene	0.0365
1,2,3,5-tetramethylbenzene	0.0510
1,3-dimethyl-4-isopropylbenzene	0.0040
1-ethyl-3-isopropylbenzene	0.0045
5-methylindane	0.0191
1-ethyl-2-propylbenzene	0.0020
OTHER C12	0.0041
1-ethyl-4-propylbenzene	0.0167
4-methylindane	0.0192
1,2,3,4-tetramethylbenzene	0.0057
1,2-dimethyl-4-propylbenzene	0.0065
1,4-diisopropylbenzene	0.0053
naphthalene	0.0410
1,3-dimethyl-5-isopropylbenzene	0.0058
1,2,3-trimethyl-4-ethylbenzene	0.0054
pentamethylbenzene	0.0035
4,7-dimethylindane	0.0012
Total	1.0000
Fraction Identified	0.9959

SD35	
Compound	Fraction
acetone	0.0047
methyl ethyl ketone	0.0029
butyl alcohol	0.1408
1-methoxy-2-propanol	0.4999
trans-1,3-dimethylcyclopentane	0.0012
methyl isobutyl ketone	0.0045
toluene	0.0026
butyl acetate	0.0113
Bz/Cl	0.0000
ethylbenzene	0.0074
m-xylene	0.0205
p-xylene	0.0076
methyl amyl ketone	0.2218
o-xylene	0.0062
ethyl-3-ethoxypropionate	0.0687
Total	1.0000
Fraction Identified	1.0000

SD36	
Compound	Fraction
methanol	0.0015
ethanol	0.0327
acetone	0.1560
2-propanol	0.0460
methyl ethyl ketone	0.0568
butyl alcohol	0.0119
cyclohexane	0.0006
2-methylhexane	0.0031
2,3-dimethylpentane	0.0015
1,1-dimethylcyclopentane	0.0009
3-methylhexane	0.0055
trans-1,3-dimethylcyclopentane	0.0042
cis-1,3-dimethylcyclopentane	0.0051
1,2-dimethylcyclopentane	0.0078
heptane	0.0209
1,2-dimethylcyclopentane	0.0024
methylcyclohexane	0.0388
1,1,3-trimethylcyclopentane	0.0039
2,5-dimethylhexane	0.0015
ethylcyclopentane	0.0033
2,4-dimethylhexane	0.0019
1,2,4-trimethylcyclopentane	0.0051
1,2,3-trimethylcyclopentane	0.0064
2,3,4-trimethylpentane	0.0004
toluene	0.0812
3-ethyl-2-methylpentane	0.0007
1,1,2-trimethylcyclopentane	0.0008
2-methylheptane	0.0034
2,3-dimethylhexane	0.0009
3-methylheptane	0.0015
3-ethylhexane	0.0006
cis-1,3-dimethylcyclohexane	0.0018
trans-1,4-dimethylcyclohexane	0.0006
butyl acetate	0.2885
octane	0.0007
Bz/Cl	0.0000
ethylbenzene	0.0234
m-xylene	0.0764
p-xylene	0.0290
o-xylene	0.0440
2-butoxyethanol	0.0095
ethyl-3-ethoxypropionate	0.0190
Total	1.0000
Fraction Identified	1.0000

SD37	
Compound	Fraction
methanol	0.0047
ethanol	0.0368
acetone	0.0023
2-propanol	0.0358
methyl ethyl ketone	0.1465
methylcyclopentane	0.0014
OTHER C7	0.0003
butyl alcohol	0.0162
cyclohexane	0.0044
2-methylhexane	0.0038
2,3-dimethylpentane	0.0023
1,1-dimethylcyclopentane	0.0020
3-methylhexane	0.0059
cis-1,3-dimethylcyclopentane	0.0071
trans-1,3-dimethylcyclopentane	0.0079
1,2-dimethylcyclopentane	0.0124
heptane	0.0133
1,2-dimethylcyclopentane	0.0008
methylcyclohexane	0.0030
1,1,3-trimethylcyclopentane	0.0222
2,5-dimethylhexane	0.0041
ethylcyclopentane	0.0007
2,4-dimethylhexane	0.0049
1,2,4-trimethylcyclopentane	0.0059
1,2,3-trimethylcyclopentane	0.0086
2,3,4-trimethylpentane	0.0004
toluene	0.0792
2,3-dimethylhexane	0.0005
OTHER C8	0.0003
3-ethyl-2-methylpentane	0.0008
1,1,2-trimethylcyclopentane	0.0025
2-methylheptane	0.0005
3,4-dimethylhexane	0.0007
3-methylheptane	0.0005
cis-1,3-dimethylcyclohexane	0.0018
trans-1,4-dimethylcyclohexane	0.0005
cis-1-ethyl-2-methylcyclopentane	0.0004
butyl acetate	0.2811
Bz/Cl	0.0000
ethylbenzene	0.0383
m-xylene	0.1019
p-xylene	0.0368
methyl amyl ketone	0.0010
o-xylene	0.0529
2-butoxyethanol	0.0015
isopropylbenzene	0.0003
ethyl-3-ethoxypropionate	0.0448
1,2,4-trimethylbenzene	0.0003
Total	1.0000
Fraction Identified	0.9997

SD38	
Compound	Fraction
2-propanol	0.0431
isobutyl alcohol	0.0013
butyl alcohol	0.0747
methylcyclohexane	0.0007
2,4-dimethylhexane	0.0003
1,2,4-trimethylcyclopentane	0.0006
1,2,3-trimethylcyclopentane	0.0005
toluene	0.0005
2,3-dimethylhexane	0.0005
1,1,2-trimethylcyclopentane	0.0003
2-methylheptane	0.0039
4-methylheptane	0.0011
3,4-dimethylhexane	0.0003
3-methylheptane	0.0027
3-ethylhexane	0.0005
cis-1,3-dimethylcyclohexane	0.0099
trans-1,4-dimethylcyclohexane	0.0034
1,1-dimethylcyclohexane	0.0009
cis-1-ethyl-3-methylcyclopentane	0.0004
trans-1-ethyl-3-methylcyclopentane	0.0004
cis-1-ethyl-2-methylcyclopentane	0.0008
trans-1,2-dimethylcyclohexane	0.0004
octane	0.0162
cis-1,4-dimethylcyclohexane	0.0005
trans-1,3-dimethylcyclohexane	0.0049
1-ethyl-1-methylcyclopentane	0.0004
2,2,5-trimethylhexane	0.0004
2,4-dimethylheptane	0.0011
cis-1,2-dimethylcyclohexane	0.0071
Added ClBz	0.0000
ethylcyclohexane	0.0070
2,5-dimethylheptane	0.0027
1,1,3-trimethylcyclohexane	0.0079
1,1,4-trimethylcyclohexane	0.0012
OTHER C9	0.0004
OTHER C9	0.0007
OTHER C9	0.0003
ethylbenzene	0.0162
trans, trans-1,2,4-trimethylcyclohexane	0.0083
trans, trans-1,3,5-trimethylcyclohexane	0.0048
m-xylene	0.0407
p-xylene	0.0158
4-methyloctane	0.0035
2-methyloctane	0.0050
methyl amyl ketone	0.1196
3-methyloctane	0.0067
1,2,3-trimethylcyclohexane	0.0005
trans, cis-1,2,4-trimethylcyclohexane	0.0053
o-xylene	0.0220
2-butoxyethanol	0.1358
cis-1-ethyl-3-methylcyclohexane	0.0058
trans-1-ethyl-3-methylcyclohexane	0.0030
cis, cis-1,2,4-trimethylcyclohexane	0.0004
isobutyl isobutyrate	0.1442
nonane	0.0179
1,2,3-trimethylcyclohexane	0.0006
cis, trans-1,2,3-trimethylcyclohexane	0.0017
trans-1-ethyl-4-methylcyclohexane	0.0061
cis-1-ethyl-4-methylcyclohexane	0.0015
2,4-dimethyloctane	0.0003
2,4,6-trimethylheptane	0.0018
isopropylcyclohexane	0.0044
2,5-dimethyloctane	0.0019
OTHER C10	0.0006
3,5-dimethyloctane	0.0012
propylcyclohexane	0.0074
2,6-dimethyloctane	0.0066
OTHER C10	0.0007
3,3,5-trimethylheptane	0.0015
OTHER C10	0.0016
3,6-dimethyloctane	0.0054
3-ethyl-2-methylheptane	0.0013
propylbenzene	0.0009
OTHER C10	0.0015
1-ethyl-3-methylbenzene	0.0010
1-ethyl-4-methylbenzene	0.0050
1,3,5-trimethylbenzene	0.0035
5-methylnonane	0.0064
4-methylnonane	0.0098
2-methylnonane	0.0022
3-ethyloctane	0.0059
3-methylnonane	0.0009
1-methyl-3-isopropylcyclohexane	0.0035
1-methyl-3-isopropylcyclohexane	0.0019
1-methyl-4-isopropylcyclohexane	0.0019
1,2-dimethyl-3-ethylcyclohexane	0.0015
1-methyl-2-isopropylcyclohexane	0.0075
1-methyl-2-isopropylcyclohexane	0.0038
1,2-dimethyl-3-ethylcyclohexane	0.0036
decane	0.0305
OTHER C11	0.0017
methyl propylcyclohexane	0.0024
methyl propylcyclohexane	0.0019
OTHER C11	0.0009
1,2,3,4-tetramethylcyclohexane	0.0010
1,2,3-trimethylbenzene	0.0036
OTHER C11	0.0008
2,5-dimethylnonane	0.0031
2,6-dimethylnonane	0.0066
OTHER C11	0.0007
OTHER C11	0.0015
methyl propylcyclohexane	0.0020
OTHER C11	0.0020
butylcyclohexane	0.0019
sec butylcyclopentane	0.0051
pentylcyclopentane	0.0023
3,7-dimethylnonane	0.0016
5-methylindane	0.0012
5-ethyl-2-methyloctane	0.0012
5-methyldecane	0.0009
4-methyldecane	0.0023
1-acetoxy-2-butoxyethane	0.0531
trans-decalin	0.0020
1,4-dimethyl-2-ethylbenzene	0.0022
3-methyldecane	0.0023
OTHER C11	0.0003
OTHER C11	0.0008
cis-decalin	0.0007
undecane	0.0040
2-methyldecalin	0.0003
OTHER C12	0.0003
Total	1.0000
Fraction Identified	0.9858

SD39	
Compound	Fraction
methylcyclohexane	0.0021
2,4-dimethylhexane	0.0011
1,2,4-trimethylcyclopentane	0.0021
1,2,3-trimethylcyclopentane	0.0020
toluene	0.0013
2,3-dimethylhexane	0.0021
1,1,2-trimethylcyclopentane	0.0013
2-methylheptane	0.0191
4-methylheptane	0.0059
3,4-dimethylhexane	0.0013
OTHER C8	0.0014
3-methylheptane	0.0139
3-ethylhexane	0.0027
cis-1,3-dimethylcyclohexane	0.0298
trans-1,4-dimethylcyclohexane	0.0111
1,1-dimethylcyclohexane	0.0032
cis-1-ethyl-3-methylcyclopentane	0.0014
trans-1-ethyl-3-methylcyclopentane	0.0014
cis-1-ethyl-2-methylcyclopentane	0.0027
trans-1,2-dimethylcyclohexane	0.0011
octane	0.0559
OTHER C9	0.0014
cis-1,4-dimethylcyclohexane	0.0131
1-ethyl-1-methylcyclopentane	0.0011
2,2,5-trimethylhexane	0.0019
2,4-dimethylheptane	0.0032
cis-1,2-dimethylcyclohexane	0.0126
Bz/Cl	0.0000
ethylcyclohexane	0.0166
2,5-dimethylheptane	0.0063
1,1,3-trimethylcyclohexane	0.0107
1,1,4-trimethylcyclohexane	0.0024
OTHER C9	0.0012
ethylbenzene	0.0103
trans, trans-1,2,4-trimethylcyclohexane	0.0233
trans, trans-1,3,5-trimethylcyclohexane	0.0099
m-xylene	0.0247
p-xylene	0.0109
4-methyloctane	0.0045
2-methyloctane	0.0062
cis-bicyclo[3.3.0]octane	0.0018
3-methyloctane	0.0067
trans, cis-1,2,4-trimethylcyclohexane	0.0147
o-xylene	0.0194
cis, trans-1,2,4-trimethylcyclohexane	0.0077
trans-1-ethyl-3-methylcyclohexane	0.0008
cis-1-ethyl-3-methylcyclohexane	0.0105
OTHER C9	0.0051
cis, cis-1,2,4-trimethylcyclohexane	0.0014
nonane	0.0102
1,2,3-trimethylcyclohexane	0.0013
cis, trans-1,2,3-trimethylcyclohexane	0.0038
trans-1-ethyl-4-methylcyclohexane	0.0107
cis-1-ethyl-4-methylcyclohexane	0.0023
2,3,5-trimethylheptane	0.0035
isopropylcyclohexane	0.0078
2,5-dimethyloctane	0.0039
3,5-dimethyloctane	0.0009
trans-bicyclo[4.3.0]nonane	0.0036
propylcyclohexane	0.0153
2,6-dimethyloctane	0.0128
3,3-dimethyloctane	0.0021
3,3,5-trimethylheptane	0.0041
3,6-dimethyloctane	0.0039
1,2-dimethyl-3-ethylcyclohexane	0.0104
3-ethyl-2-methylheptane	0.0054
propylbenzene	0.0023
OTHER C10	0.0035
1-ethyl-3-methylbenzene	0.0114
1-ethyl-4-methylbenzene	0.0157
1,3,5-trimethylbenzene	0.0028
5-methylnonane	0.0220
4-methylnonane	0.0232
2-methylnonane	0.0058
1-ethyl-2-methylbenzene	0.0154
3-ethyloctane	0.0020
1-methyl-3-isopropylcyclohexane	0.0087
1-methyl-3-isopropylcyclohexane	0.0058
1-methyl-4-isopropylcyclohexane	0.0051
1-methyl-2-isopropylcyclohexane	0.0029
1,2,4-trimethylbenzene	0.0318
1,2-dimethyl-3-ethylcyclohexane	0.0113
1,2-dimethyl-3-ethylcyclohexane	0.0072
decane	0.0550
methyl propylcyclohexane	0.0041
diethylcyclohexane	0.0053
methyl propylcyclohexane	0.0051
diethylcyclohexane	0.0021
2-ethyl-1,3-dimethylcyclohexane	0.0030
1,2,3-trimethylbenzene	0.0069
sec butylcyclohexane	0.0078
2,5-dimethylnonane	0.0075
2,6-dimethylnonane	0.0169
3,6-dimethylnonane	0.0084
isobutylcyclohexane	0.0055
methyl propylcyclohexane	0.0050
butylcyclohexane	0.0122
4,5-dimethylnonane	0.0061
3,7-dimethylnonane	0.0059
4-ethylnonane	0.0057
1-ethyl-2,2,6-trimethylcyclohexane	0.0036
5-methyldecane	0.0116
4-methyldecane	0.0066
trans-decalin	0.0077
3-ethylnonane	0.0094
3-methyldecane	0.0096
1,1-dimethyl-2-propylcyclohexane	0.0022
ethyl propylcyclohexane	0.0019
ethyl propylcyclohexane	0.0023
1,2-diethyl-1-methylcyclohexane	0.0044
diethylcyclohexane	0.0019
cis-decalin	0.0081
methyl butylcyclohexane	0.0017
undecane	0.0360
2-methyldecalin	0.0063
2-methyldecalin	0.0056
ethyl propylcyclohexane	0.0023
2,5-dimethyldecane	0.0057
5-ethyl-3-methyloctane	0.0067
pentylcyclohexane	0.0042
hexylcyclopentane	0.0039
6-methylundecane	0.0027
5-methylundecane	0.0016
4-methylundecane	0.0026
2-methylundecane	0.0033
3-methylundecane	0.0033
dodecane	0.0105
2,6-dimethylundecane	0.0013
Total	1.0000
Fraction Identified	0.9874

SD40	
Compound	Fraction
methylcyclohexane	0.0018
toluene	0.0024
3,4-dimethylhexane	0.0023
cis-1,3-dimethylcyclohexane	0.0019
octane	0.0050
cis-1,2-dimethylcyclohexane	0.0017
Chlorobenzene (added)	0.0000
ethylcyclohexane	0.0029
1,1,3-trimethylcyclohexane	0.0020
ethylbenzene	0.0030
trans, trans-1,2,4-trimethylcyclohexane	0.0024
2,3-dimethylheptane	0.0015
m-xylene	0.0123
p-xylene	0.0035
4-methyloctane	0.0054
3-methyloctane	0.0039
1,2,3-trimethylcyclohexane	0.0021
o-xylene	0.0064
cis, trans-1,2,4-trimethylcyclohexane	0.0023
cis-1-ethyl-3-methylcyclohexane	0.0052
trans-1-ethyl-3-methylcyclohexane	0.0028
nonane	0.0263
cis, trans-1,2,3-trimethylcyclohexane	0.0014
trans-1-ethyl-4-methylcyclohexane	0.0053
cis-1-ethyl-4-methylcyclohexane	0.0013
isopropylbenzene	0.0030
isopropylcyclohexane	0.0063
2,5-dimethyloctane	0.0033
cis-1-ethyl-2-methylcyclohexane	0.0029
propylcyclohexane	0.0125
2,6-dimethyloctane	0.0104
butylcyclopentane	0.0030
3,6-dimethyloctane	0.0028
1,1,2,3-tetramethylcyclohexane	0.0066
propylbenzene	0.0048
OTHER C10	0.0015
1-ethyl-1,3-dimethylcyclohexane	0.0022
1-ethyl-3-methylbenzene	0.0114
1-ethyl-4-methylbenzene	0.0126
1,3,5-trimethylbenzene	0.0289
2-methylnonane	0.0202
3-ethyloctane	0.0043
1-methyl-2-ethylbenzene	0.0157
1-methyl-4-isopropylcyclohexane	0.0070
1-methyl-3-isopropylcyclohexane	0.0016
1-methyl-3-isopropylcyclohexane	0.0028
2-ethyl-1,3-dimethylcyclohexane	0.0036
diethylcyclohexane	0.0020
1,2,4-trimethylbenzene	0.0402
1-methyl-2-isopropylcyclohexane	0.0098
1,2-dimethyl-3-ethylcyclohexane	0.0067
decane	0.0992
methyl propylcyclohexane	0.0034
methyl propylcyclohexane	0.0060
methyl propylcyclohexane	0.0074
2-ethyl-1,3-dimethylcyclohexane	0.0022
1-methyl-3-isopropylbenzene	0.0101
1,2,3-trimethylbenzene	0.0220
1-methyl-4-isopropylbenzene	0.0067
2,6-dimethylnonane	0.0287
methyl propylcyclohexane	0.0121
isobutylcyclohexane	0.0068
1-methyl-2-isopropylbenzene	0.0083
pentylcyclopentane	0.0186
3,7-dimethylnonane	0.0080
1,3-diethylbenzene	0.0047
1-methyl-3-propylbenzene	0.0139
1,3-dimethyl-5-ethylbenzene	0.0196
4-ethylnonane	0.0046
5-methyldecane	0.0185
4-methyldecane	0.0117
2-methyldecane	0.0214
3-methyldecane	0.0172
1,4-dimethyl-2-ethylbenzene	0.0189
1,3-dimethyl-4-ethylbenzene	0.0059
1,1-dimethyl-2-propylcyclohexane	0.0025
1,2-dimethyl-4-ethylbenzene	0.0124
1,3-dimethyl-2-ethylbenzene	0.0066
diethylcyclohexane	0.0042
methyl butylcyclohexane	0.0105
undecane	0.1195
1-ethyl-4-isopropylbenzene	0.0045
2-methyldecalin	0.0080
diethylcyclohexane	0.0062
2,4-dimethyldecane	0.0053
1,2,3,5-tetramethylbenzene	0.0143
2-methyldecalin	0.0026
4,5-dimethyldecane	0.0108
OTHER C12	0.0018
2,7-dimethyldecane	0.0019
Indan/5Me	0.0050
pentylcyclohexane	0.0070
4-methylindane	0.0064
1,2,3,4-tetramethylbenzene	0.0020
5-methylundecane	0.0087
4-methylundecane	0.0035
2-methylundecane	0.0085
1,4-diisopropylbenzene	0.0039
naphthalene	0.0090
dodecane	0.0230
2,6-dimethylundecane	0.0025
tridecane	0.0015
Total	1.0000
Fraction Identified	0.9967

SD41	
Compound	Fraction
2,4-dimethylpentane	0.0014
toluene	0.0013
4-methylheptane	0.0013
3,4-dimethylhexane	0.0030
octane	0.0024
1-propoxy-2-propanol	0.1082
Added ClBz	0.0000
1,1,3-trimethylcyclohexane	0.0037
ethylbenzene	0.0109
trans, trans-1,3,5-trimethylcyclohexane	0.0022
m-xylene	0.0184
p-xylene	0.0067
4-methyloctane	0.0040
3-methyloctane	0.0035
1,2,3-trimethylcyclohexane	0.0027
o-xylene	0.0071
cis, trans-1,2,4-trimethylcyclohexane	0.0030
OTHER C9	0.0013
cis-1-ethyl-3-methylcyclohexane	0.0046
trans-1-ethyl-4-methylcyclohexane	0.0026
nonane	0.0268
trans-1-ethyl-3-methylcyclohexane	0.0011
cis, trans-1,2,3-trimethylcyclohexane	0.0018
trans-1-ethyl-2-methylcyclohexane	0.0069
isopropylbenzene	0.0019
3,4-dimethyloctane	0.0048
isopropylcyclohexane	0.0069
2,5-dimethyloctane	0.0057
3,5-dimethyloctane	0.0013
cis-1-ethyl-2-methylcyclohexane	0.0040
propylcyclohexane	0.0142
2,6-dimethyloctane	0.0169
3,3,5-trimethylheptane	0.0039
3,6-dimethyloctane	0.0045
5-ethyl-2-methylheptane	0.0109
propylbenzene	0.0056
1,1,2,3-tetramethylcyclohexane	0.0024
2,3-dimethyloctane	0.0033
1-ethyl-3-methylbenzene	0.0103
1-ethyl-4-methylbenzene	0.0171
3-ethyl-4-methylheptane	0.0018
1,3,5-trimethylbenzene	0.0334
4-methylnonane	0.0311
3-methylnonane	0.0065
1-ethyl-2-methylbenzene	0.0237
1-methyl-4-isopropylcyclohexane	0.0023
methyl isopropylcyclohexane	0.0093
1-methyl-3-isopropylcyclohexane	0.0053
1,2-dimethyl-3-ethylcyclohexane	0.0043
diethylcyclohexane	0.0028
1,2,4-trimethylbenzene	0.0355
methyl propylcyclohexane	0.0103
methyl propylcyclohexane	0.0070
decane	0.1018
methyl propylcyclohexane	0.0039
methyl propylcyclohexane	0.0064
1,4-dimethyl-1-ethylcyclohexane	0.0086
2-ethyl-1,3-dimethylcyclohexane	0.0031
1-methyl-3-isopropylbenzene	0.0112
1,2,3-trimethylbenzene	0.0105
2,5-dimethylnonane	0.0106
2,6-dimethylnonane	0.0225
methyl propylcyclohexane	0.0115
isobutylcyclohexane	0.0056
pentylcyclopentane	0.0079
butylcyclohexane	0.0149
3,7-dimethylnonane	0.0082
1,3-diethylbenzene	0.0038
1-methyl-3-propylbenzene	0.0104
1,3-dimethyl-5-ethylbenzene	0.0121
5-ethyl-2-methyloctane	0.0046
5-methyldecane	0.0177
4-methyldecane	0.0111
2-methyldecane	0.0157
trans-decalin	0.0102
3-methyldecane	0.0154
ethyl propylcyclohexane	0.0029
ethyl propylcyclohexane	0.0023
ethyl propylcyclohexane	0.0067
methyl butylcyclohexane	0.0039
ethyl propylcyclohexane	0.0024
methyl butylcyclohexane	0.0074
undecane	0.0563
1,2-dimethyl-3-ethylbenzene	0.0028
1-ethyl-4-isopropylbenzene	0.0051
2-methyldecalin	0.0064
1,2,4,5-tetramethylbenzene	0.0028
2,6-dimethyldecane	0.0081
2-methyldecalin	0.0024
OTHER C12	0.0067
5-methylindane	0.0015
isopentylcyclohexane	0.0023
pentylcyclohexane	0.0051
hexylcyclopentane	0.0033
6-methylundecane	0.0031
5-methylundecane	0.0021
4-methylundecane	0.0028
2-methylundecane	0.0041
3-methylundecane	0.0036
naphthalene	0.0041
dodecane	0.0106
2,6-dimethylundecane	0.0012
Total	1.0000
Fraction Identified	0.9919

SD42	
Compound	Fraction
3,4-dimethylhexane	0.0019
octane	0.0012
cis-1,2-dimethylcyclohexane	0.0009
Bz/Cl	0.0000
ethylcyclohexane	0.0010
1,1,3-trimethylcyclohexane	0.0010
ethylbenzene	0.0046
trans, trans-1,2,4-trimethylcyclohexane	0.0025
2,3-dimethylheptane	0.0012
m-xylene	0.0105
p-xylene	0.0038
4-methyloctane	0.0035
3-methyloctane	0.0030
1,2,3-trimethylcyclohexane	0.0025
o-xylene	0.0049
cis, trans-1,2,4-trimethylcyclohexane	0.0013
trans-1-ethyl-3-methylcyclohexane	0.0012
cis-1-ethyl-3-methylcyclohexane	0.0038
trans-1-ethyl-3-methylcyclohexane	0.0019
nonane	0.0170
cis, trans-1,2,3-trimethylcyclohexane	0.0014
2,4-dimethyloctane	0.0051
cis-1-ethyl-4-methylcyclohexane	0.0012
isopropylbenzene	0.0020
OTHER C10	0.0040
2,5-dimethyloctane	0.0023
cis-1-ethyl-2-methylcyclohexane	0.0016
propylcyclohexane	0.0081
2,6-dimethyloctane	0.0082
butylcyclopentane	0.0020
3,6-dimethyloctane	0.0021
1,1,2,3-tetramethylcyclohexane	0.0068
propylbenzene	0.0023
cyclohexane/1124Me4	0.0011
2,3-dimethyloctane	0.0014
1-ethyl-3-methylbenzene	0.0038
1-ethyl-4-methylbenzene	0.0074
1,3,5-trimethylbenzene	0.0048
4-methylnonane	0.0100
2-methylnonane	0.0146
3-ethyloctane	0.0032
1-methyl-2-ethylbenzene	0.0102
1-methyl-3-isopropylcyclohexane	0.0046
1-methyl-3-isopropylcyclohexane	0.0031
2-ethyl-1,3-dimethylcyclohexane	0.0029
diethylcyclohexane	0.0019
1,2,4-trimethylbenzene	0.0173
1-methyl-2-isopropylcyclohexane	0.0064
1,2-dimethyl-3-ethylcyclohexane	0.0047
decane	0.0533
methyl propylcyclohexane	0.0030
methyl propylcyclohexane	0.0043
methyl propylcyclohexane	0.0038
diethylcyclohexane	0.0015
2-ethyl-1,3-dimethylcyclohexane	0.0018
2,5-dimethylnonane	0.0071
1,2,3-trimethylbenzene	0.0050
3,5-dimethylnonane	0.0075
2,6-dimethylnonane	0.0196
isopropylcyclohexane	0.0104
isobutylcyclohexane	0.0058
butylcyclohexane	0.0072
pentylcyclopentane	0.0157
3,7-dimethylnonane	0.0107
ethyl propylcyclohexane	0.0032
OTHER C11	0.0089
1,3-dimethyl-5-ethylbenzene	0.0081
OTHER C11	0.0066
5-methyldecane	0.0232
4-methyldecane	0.0159
2-methyldecane	0.0188
2,3-dimethylnonane	0.0028
trans-decalin	0.0194
3-methyldecane	0.0239
1,1-dimethyl-2-propylcyclohexane	0.0052
ethyl propylcyclohexane	0.0042
ethyl propylcyclohexane	0.0050
ethyl propylcyclohexane	0.0086
ethyl propylcyclohexane	0.0044
cis-decalin	0.0196
ethyl propylcyclohexane	0.0069
ethyl propylcyclohexane	0.0049
undecane	0.1209
2-methyldecalin	0.0197
4,6-dimethyldecane	0.0184
2,4-dimethyldecane	0.0067
3,6-dimethyldecane	0.0203
2,6-dimethyldecane	0.0071
2-methyldecalin	0.0071
4,5-dimethyldecane	0.0249
5-sec butylnonane	0.0028
(2-methylbutyl)cyclohexane	0.0050
isopentylcyclohexane	0.0067
pentylcyclohexane	0.0202
hexylcyclopentane	0.0129
OTHER C12	0.0045
6-methylundecane	0.0106
5-methylundecane	0.0088
4-methylundecane	0.0139
2-methylundecane	0.0158
OTHER C12	0.0030
3-methylundecane	0.0162
OTHER C12	0.0045
methyl pentylcyclohexane	0.0038
naphthalene	0.0041
methyl pentylcyclohexane	0.0022
methyl pentylcyclohexane	0.0029
methyl pentylcyclohexane	0.0070
dodecane	0.0554
2,4-dimethylundecane	0.0041
methyl pentylcyclohexane	0.0018
2,6-dimethylundecane	0.0074
OTHER C13	0.0010
hexylcyclohexane	0.0017
Total	1.0000
Fraction Identified	0.9675

SD43	
Compound	Fraction
3,4-dimethylhexane	0.0013
octane	0.0020
cis-1,2-dimethylcyclohexane	0.0011
Bz/Cl	0.0000
ethylcyclohexane	0.0013
1,1,3-trimethylcyclohexane	0.0011
ethylbenzene	0.0085
trans, trans-1,2,4-trimethylcyclohexane	0.0032
2,3-dimethylheptane	0.0016
m-xylene	0.0209
p-xylene	0.0080
4-methyloctane	0.0050
3-methyloctane	0.0044
1,2,3-trimethylcyclohexane	0.0034
o-xylene	0.0092
cis, trans-1,2,4-trimethylcyclohexane	0.0018
OTHER C9	0.0018
cis-1-ethyl-3-methylcyclohexane	0.0018
cis-1-ethyl-4-methylcyclohexane	0.0078
trans-1-ethyl-3-methylcyclohexane	0.0047
nonane	0.0324
trans-1-ethyl-2-methylcyclohexane	0.0017
cis, trans-1,2,3-trimethylcyclohexane	0.0034
2,4-dimethyloctane	0.0147
OTHER C10	0.0036
3,4-dimethyloctane	0.0010
isopropylbenzene	0.0057
OTHER C10	0.0017
isopropylcyclohexane	0.0095
2,5-dimethyloctane	0.0067
3,5-dimethyloctane	0.0016
cis-1-ethyl-2-methylcyclohexane	0.0052
propylcyclohexane	0.0256
2,6-dimethyloctane	0.0277
3,3,5-trimethylheptane	0.0025
butylcyclopentane	0.0053
3,6-dimethyloctane	0.0065
2,3-dimethyloctane	0.0167
3-ethyl-2-methylheptane	0.0037
OTHER C10	0.0039
4-ethyloctane	0.0051
1-ethyl-3-methylbenzene	0.0020
1-ethyl-4-methylbenzene	0.0164
5-methylnonane	0.0114
4-methylnonane	0.0204
2-methylnonane	0.0386
3-ethyloctane	0.0091
3-methylnonane	0.0180
1-methyl-4-isopropylcyclohexane	0.0034
1-methyl-3-isopropylcyclohexane	0.0126
1-methyl-3-isopropylcyclohexane	0.0085
2-ethyl-1,3-dimethylcyclohexane	0.0077
methyl isopropylcyclohexane	0.0072
methyl isopropylcyclohexane	0.0220
methyl propylcyclohexane	0.0162
1,2-dimethyl-3-ethylcyclohexane	0.0127
decane	0.0989
methyl propylcyclohexane	0.0061
methyl propylcyclohexane	0.0104
methyl propylcyclohexane	0.0076
diethylcyclohexane	0.0036
2-ethyl-1,3-dimethylcyclohexane	0.0047
2,5-dimethylnonane	0.0130
OTHER C10	0.0042
3,5-dimethylnonane	0.0115
2,6-dimethylnonane	0.0304
6-ethyl-2-methyloctane	0.0030
2,7-dimethylnonane	0.0077
OTHER C10	0.0067
isobutylcyclohexane	0.0084
butylcyclohexane	0.0082
pentylcyclopentane	0.0169
3,7-dimethylnonane	0.0143
OTHER C11	0.0034
methyl propylcyclohexane	0.0082
1,3-dimethyl-5-ethylbenzene	0.0072
4-ethylnonane	0.0061
4-ethylnonane	0.0045
5-methyldecane	0.0165
4-methyldecane	0.0138
2-methyldecane	0.0135
ethyl propylcyclohexane	0.0137
3-methyldecane	0.0174
1,1-dimethyl-2-propylcyclohexane	0.0031
ethyl propylcyclohexane	0.0028
ethyl propylcyclohexane	0.0031
OTHER C11	0.0058
ethyl propylcyclohexane	0.0030
methyl butylcyclohexane	0.0117
cis-decalin	0.0027
undecane	0.0610
2-methyldecalin	0.0099
4,6-dimethyldecane	0.0082
2,6-dimethyldecane	0.0030
3,6-dimethyldecane	0.0082
OTHER C12	0.0026
3-methylnonane	0.0080
OTHER C12	0.0014
pentylcyclohexane	0.0056
3-ethyldecane	0.0028
6-methylundecane	0.0027
5-methylundecane	0.0018
4-methylundecane	0.0029
2-methylundecane	0.0025
3-methylundecane	0.0031
dodecane	0.0049
Total	1.0000
Fraction Identified	0.9648

SD44	
Compound	Fraction
methylcyclopentane	0.0011
methylcyclohexane	0.0046
1,1,3-trimethylcyclopentane	0.0011
2,5-dimethylhexane	0.0013
2,4-dimethylhexane	0.0024
1,2,4-trimethylcyclopentane	0.0039
1,2,3-trimethylcyclopentane	0.0035
2,3-dimethylhexane	0.0037
3-ethyl-2-methylpentane	0.0010
2-methylheptane	0.0320
4-methylheptane	0.0100
3,4-dimethylhexane	0.0027
OTHER C8	0.0013
3-methylheptane	0.0268
3-ethylhexane	0.0055
OTHER C8	0.0008
cis-1,3-dimethylcyclohexane	0.0353
trans-1,4-dimethylcyclohexane	0.0130
OTHER C8	0.0009
1,1-dimethylcyclohexane	0.0036
OTHER C8	0.0020
trans-1-ethyl-3-methylcyclopentane	0.0020
cis-1-ethyl-2-methylcyclopentane	0.0034
trans-1,2-dimethylcyclohexane	0.0013
octane	0.0705
cis-1,4-dimethylcyclohexane	0.0015
trans-1,3-dimethylcyclohexane	0.0155
OTHER C9	0.0013
OTHER C9	0.0013
2,2,5-trimethylhexane	0.0033
2,4-dimethylheptane	0.0057
2,6-dimethylheptane	0.0148
Added ClBz	0.0000
ethylcyclohexane	0.0184
2,5-dimethylheptane	0.0079
1,1,3-trimethylcyclohexane	0.0108
1,1,4-trimethylcyclohexane	0.0027
OTHER C9	0.0013
ethylbenzene	0.0092
trans, trans-1,2,4-trimethylcyclohexane	0.0225
2,3-dimethylheptane	0.0067
1,2,4-trimethylcyclohexane	0.0031
m-xylene	0.0212
p-xylene	0.0093
4-methyloctane	0.0114
OTHER C9	0.0017
3-methyloctane	0.0067
1,2,3-trimethylcyclohexane	0.0145
o-xylene	0.0164
cis, trans-1,2,4-trimethylcyclohexane	0.0071
cis-1-ethyl-3-methylcyclohexane	0.0106
trans-1-ethyl-3-methylcyclohexane	0.0046
nonane	0.0106
trans-1-ethyl-2-methylcyclohexane	0.0008
cis, trans-1,2,3-trimethylcyclohexane	0.0041
trans-1-ethyl-4-methylcyclohexane	0.0106
cis-1-ethyl-4-methylcyclohexane	0.0021
3,4-dimethyloctane	0.0015
isopropylbenzene	0.0030
OTHER C10	0.0014
isopropylcyclohexane	0.0053
2,5-dimethyloctane	0.0036
3,5-dimethyloctane	0.0008
cis-1-ethyl-2-methylcyclohexane	0.0039
propylcyclohexane	0.0154
2,6-dimethyloctane	0.0123
butylcyclopentane	0.0053
3,6-dimethyloctane	0.0037
1,1,2,3-tetramethylcyclohexane	0.0101
propylbenzene	0.0048
OTHER C10	0.0020
2,3-dimethyloctane	0.0031
1-ethyl-3-methylbenzene	0.0106
1-ethyl-4-methylbenzene	0.0155
1,3,5-trimethylbenzene	0.0255
2-methylnonane	0.0138
3-ethyloctane	0.0095
OTHER C10	0.0059
1-methyl-2-ethylbenzene	0.0156
OTHER C10	0.0016
methyl propylcyclohexane	0.0085
1-methyl-3-isopropylcyclohexane	0.0054
methyl propylcyclohexane	0.0133
1,2,4-trimethylbenzene	0.0398
methyl propylcyclohexane	0.0102
1,2-dimethyl-3-ethylcyclohexane	0.0066
decane	0.0594
diethylcyclohexane	0.0036
diethylcyclohexane	0.0049
diethylcyclohexane	0.0047
diethylcyclohexane	0.0017
2-ethyl-1,3-dimethylcyclohexane	0.0015
2,5-dimethylnonane	0.0065
1,2,3-trimethylbenzene	0.0079
3,5-dimethylnonane	0.0054
2,6-dimethylnonane	0.0138
methyl propylcyclohexane	0.0076
2,7-dimethylnonane	0.0044
butylcyclohexane	0.0039
pentylcyclopentane	0.0097
3,7-dimethylnonane	0.0049
methyl propylcyclohexane	0.0035
4-ethylnonane	0.0030
OTHER C11	0.0024
OTHER C11	0.0014
5-methyldecane	0.0057
4-methyldecane	0.0053
2-methyldecane	0.0054
trans-decalin	0.0078
3-methyldecane	0.0058
1,1-dimethyl-2-propylcyclohexane	0.0009
OTHER C11	0.0008
OTHER C11	0.0010
cis-decalin	0.0038
undecane	0.0259
2-methyldecalin	0.0023
4,6-dimethyldecane	0.0020
3,6-dimethyldecane	0.0036
2-methyldecalin	0.0013
2,7-dimethyldecane	0.0043
pentylcyclohexane	0.0036
hexylcyclopentane	0.0020
6-methylundecane	0.0016
5-methylundecane	0.0013
4-methylundecane	0.0017
2-methylundecane	0.0025
3-methylundecane	0.0027
dodecane	0.0074
2,6-dimethylundecane	0.0009
Total	1.0000
Fraction Identified	0.9738

SD45	
Compound	Fraction
4-methylheptane	0.0021
octane	0.0019
Added ClBz	0.0000
ethylbenzene	0.0021
trans, trans-1,2,4-trimethylcyclohexane	0.0014
m-xylene	0.0074
p-xylene	0.0022
4-methyloctane	0.0022
3-methyloctane	0.0018
1,2,3-trimethylcyclohexane	0.0015
1,2,3-trimethylcyclohexane	0.0038
cis-1-ethyl-3-methylcyclohexane	0.0028
trans-1-ethyl-3-methylcyclohexane	0.0013
nonane	0.0109
trans-1-ethyl-4-methylcyclohexane	0.0035
2,3,5-trimethylheptane	0.0014
isopropylcyclohexane	0.0027
3,5-dimethyloctane	0.0018
cis-1-ethyl-2-methylcyclohexane	0.0015
propylcyclohexane	0.0068
2,6-dimethyloctane	0.0066
butylcyclopentane	0.0027
3,6-dimethyloctane	0.0018
1,1,2,3-tetramethylcyclohexane	0.0044
propylbenzene	0.0024
1-ethyl-3-methylbenzene	0.0056
1-ethyl-4-methylbenzene	0.0074
4-methylnonane	0.0159
2-methylnonane	0.0063
1,3,5-trimethylbenzene	0.0047
OTHER C10	0.0025
3-methylnonane	0.0064
1-ethyl-2-methylbenzene	0.0027
methyl isopropylcyclohexane	0.0037
1-methyl-3-isopropylcyclohexane	0.0026
2-ethyl-1,3-dimethylcyclohexane	0.0021
1,2,4-trimethylbenzene	0.0331
1-methyl-2-isopropylcyclohexane	0.0049
1,2-dimethyl-3-ethylcyclohexane	0.0034
decane	0.0406
sec butylbenzene	0.0018
methyl propylcyclohexane	0.0030
methyl propylcyclohexane	0.0035
1-methyl-3-isopropylbenzene	0.0031
1,2,3-trimethylbenzene	0.0139
2,5-dimethylnonane	0.0028
2,6-dimethylnonane	0.0107
methyl propylcyclohexane	0.0035
isobutylcyclohexane	0.0017
butylcyclohexane	0.0025
pentylcyclopentane	0.0066
3,7-dimethylnonane	0.0037
OTHER C11	0.0020
methyl propylcyclohexane	0.0059
1,3-dimethyl-5-ethylbenzene	0.0118
5-methyldecane	0.0104
trans-decalin	0.0052
4-methyldecane	0.0094
2-methyldecane	0.0148
3-methyldecane	0.0178
1,4-dimethyl-2-ethylbenzene	0.0217
1,3-dimethyl-4-ethylbenzene	0.0046
1,1-dimethyl-2-propylcyclohexane	0.0059
1-methylindane	0.0050
1,2-dimethyl-4-ethylbenzene	0.0146
1,3-dimethyl-2-ethylbenzene	0.0101
ethyl propylcyclohexane	0.0077
methyl butylcyclohexane	0.0279
cis-decalin	0.0061
undecane	0.1509
2-methyldecalin	0.0294
1-ethyl-4-isopropylbenzene	0.0117
OTHER C12	0.0073
1,2,4,5-tetramethylbenzene	0.0149
3,6-dimethyldecane	0.0338
2-methyldecalin	0.0160
2,6-dimethyldecane	0.0332
5-sec-butylnonane	0.0051
1-ethyl-3-isopropylbenzene	0.0070
5-methylindane	0.0104
pentylcyclohexane	0.0238
hexylcyclopentane	0.0153
1,2,3,4-tetramethylbenzene	0.0067
5-methylundecane	0.0257
4-methylundecane	0.0145
2-methylundecane	0.0199
OTHER C12	0.0035
3-methylundecane	0.0186
3,8-dimethyldecane	0.0079
methyl pentylcyclohexane	0.0047
naphthalene	0.0095
methyl pentylcyclohexane	0.0048
5,6-dimethylindane	0.0064
dodecane	0.0464
butyl ethylcyclohexane	0.0038
butyl ethylcyclohexane	0.0038
2,6-dimethylundecane	0.0071
2,9-dimethylundecane	0.0013
Total	1.0000
Fraction Identified	0.9847

SD46	
Compound	Fraction
1,2-dimethylcyclopentane	0.0005
2,3,4-trimethylpentane	0.0005
OTHER C8	0.0007
1,1,2-trimethylcyclopentane	0.0009
3-methylheptane	0.0020
3,4-dimethylhexane	0.0006
3-ethylhexane	0.0010
octane	0.0027
cis-1,2-dimethylcyclohexane	0.0011
Bz/Cl	0.0000
ethylcyclohexane	0.0013
2,5-dimethylheptane	0.0005
1,1,3-trimethylcyclohexane	0.0014
ethylbenzene	0.0030
trans, trans-1,2,4-trimethylcyclohexane	0.0027
2,3-dimethylheptane	0.0011
m-xylene	0.0103
p-xylene	0.0035
4-methyloctane	0.0032
3-methyloctane	0.0024
1,2,3-trimethylcyclohexane	0.0024
o-xylene	0.0051
cis, trans-1,2,4-trimethylcyclohexane	0.0011
OTHER C9	0.0010
cis-1-ethyl-3-methylcyclohexane	0.0006
cis-1-ethyl-3-methylcyclohexane	0.0040
cis, cis-1,2,4-trimethylcyclohexane	0.0021
nonane	0.0154
trans-1-ethyl-2-methylcyclohexane	0.0007
cis, trans-1,2,3-trimethylcyclohexane	0.0015
2,4-dimethyloctane	0.0052
cis-1-ethyl-4-methylcyclohexane	0.0012
3,4-dimethyloctane	0.0026
isopropylcyclohexane	0.0049
2,5-dimethyloctane	0.0029
3,5-dimethyloctane	0.0006
cis-1-ethyl-2-methylcyclohexane	0.0025
propylcyclohexane	0.0105
2,6-dimethyloctane	0.0097
3,3,5-trimethylheptane	0.0013
butylcyclopentane	0.0028
3,6-dimethyloctane	0.0027
1,1,2,3-tetramethylcyclohexane	0.0068
3-ethyl-2-methylheptane	0.0030
OTHER C10	0.0015
OTHER C10	0.0021
1-ethyl-3-methylbenzene	0.0056
1-ethyl-4-methylbenzene	0.0096
1,3,5-trimethylbenzene	0.0017
4-methylnonane	0.0189
2-methylnonane	0.0178
3-ethyloctane	0.0040
3-methylnonane	0.0115
1-methyl-4-isopropylcyclohexane	0.0011
1-methyl-3-isopropylcyclohexane	0.0061
1-methyl-3-isopropylcyclohexane	0.0040
2-ethyl-1,3-dimethylcyclohexane	0.0035
1-ethyl-1,2-dimethylcyclohexane	0.0020
1-methyl-2-isopropylcyclohexane	0.0224
1-methyl-2-isopropylcyclohexane	0.0087
1,2-dimethyl-3-ethylcyclohexane	0.0057
decane	0.0712
ethyl propylcyclohexane	0.0048
ethyl propylcyclohexane	0.0059
2-ethyl-1,3-dimethylcyclohexane	0.0023
2,4-dimethylnonane	0.0075
1,2,3-trimethylbenzene	0.0080
sec butylcyclohexane	0.0038
2,5-dimethylnonane	0.0050
2,6-dimethylnonane	0.0248
OTHER C11	0.0015
methyl propylcyclohexane	0.0094
isobutylcyclohexane	0.0056
butylcyclohexane	0.0070
pentylcyclopentane	0.0158
3,7-dimethylnonane	0.0091
OTHER C11	0.0035
ethyl propylcyclohexane	0.0094
1,3-dimethyl-5-ethylbenzene	0.0110
5-ethyl-2-methyloctane	0.0053
5-methyldecane	0.0216
4-methyldecane	0.0129
2-methyldecane	0.0190
5-isopropylnonane	0.0019
1,4-dimethyl-2-ethylbenzene	0.0154
3-methyldecane	0.0184
1,3-dimethyl-4-ethylbenzene	0.0038
1,1-dimethyl-2-propylcyclohexane	0.0043
1,3-dimethyl-2-ethylbenzene	0.0055
diethylcyclohexane	0.0062
diethylcyclohexane	0.0072
ethyl propylcyclohexane	0.0060
methyl butylcyclohexane	0.0215
cis-decalin	0.0038
ethyl propylcyclohexane	0.0038
undecane	0.1336
OTHER C12	0.0059
6-ethyl-2-methyloctane	0.0122
2-methyldecalin	0.0090
4,6-dimethyldecane	0.0068
2,4-dimethyldecane	0.0063
3,6-dimethyldecane	0.0248
2-methyldecalin	0.0057
4,5-dimethyldecane	0.0215
OTHER C12	0.0035
OTHER C12	0.0040
5-methylindane	0.0071
pentylcyclohexane	0.0146
hexylcyclopentane	0.0138
OTHER C12	0.0037
6-methylundecane	0.0163
4-methylundecane	0.0095
2-methylundecane	0.0137
OTHER C12	0.0019
3-methylundecane	0.0100
OTHER C12	0.0026
methyl pentylcyclohexane	0.0016
naphthalene	0.0090
methyl pentylcyclohexane	0.0022
OTHER C12	0.0016
OTHER C12	0.0018
dodecane	0.0330
OTHER C13	0.0016
2,6-dimethylundecane	0.0036
hexylcyclohexane	0.0009
Total	1.0000
Fraction Identified	0.9632

SD47	
Compound	Fraction
3,4-dimethylhexane	0.0032
Added ClBz	0.0000
1,1,3-trimethylcyclohexane	0.0033
ethylbenzene	0.0040
trans, trans-1,2,4-trimethylcyclohexane	0.0069
trans, trans-1,3,5-trimethylcyclohexane	0.0026
m-xylene	0.0085
p-xylene	0.0033
4-methyloctane	0.0031
3-ethylheptane	0.0030
3-methyloctane	0.0015
1,2,3-trimethylcyclohexane	0.0081
o-xylene	0.0084
1,1,2-trimethylcyclohexane	0.0025
cis, trans-1,2,4-trimethylcyclohexane	0.0035
OTHER C9	0.0020
cis-1-ethyl-3-methylcyclohexane	0.0078
trans-1-ethyl-3-methylcyclohexane	0.0048
nonane	0.0169
1,2,3-trimethylcyclohexane	0.0037
cis, trans-1,2,3-trimethylcyclohexane	0.0046
trans-1-ethyl-4-methylcyclohexane	0.0127
isopropylbenzene	0.0026
2,3,5-trimethylheptane	0.0042
isopropylcyclohexane	0.0146
2,5-dimethyloctane	0.0048
2,7-dimethyloctane	0.0045
propylcyclohexane	0.0199
2,6-dimethyloctane	0.0175
3,3,5-trimethylheptane	0.0028
2,2,3,3-tetramethylpentane	0.0057
3,6-dimethyloctane	0.0049
1,2-dimethyl-3-ethylcyclohexane	0.0126
3-ethyl-2-methylheptane	0.0065
propylbenzene	0.0027
1,1,2,3-tetramethylcyclohexane	0.0046
1-ethyl-3-methylbenzene	0.0094
1-ethyl-4-methylbenzene	0.0160
1,3,5-trimethylbenzene	0.0041
4-methylnonane	0.0225
2-methylnonane	0.0304
1-ethyl-1,3-dimethylcyclohexane	0.0073
1-ethyl-2-methylbenzene	0.0153
diethylcyclohexane	0.0038
methyl isopropylcyclohexane	0.0113
1-methyl-3-isopropylcyclohexane	0.0095
1,2-dimethyl-3-ethylcyclohexane	0.0070
diethylcyclohexane	0.0041
1,2,4-trimethylbenzene	0.0291
1-methyl-2-isopropylcyclohexane	0.0146
1-methyl-2-isopropylcyclohexane	0.0106
decane	0.0639
methyl propylcyclohexane	0.0053
methyl propylcyclohexane	0.0067
methyl propylcyclohexane	0.0066
diethylcyclohexane	0.0024
diethylcyclohexane	0.0016
1-methyl-3-isopropylbenzene	0.0027
1,3-dimethyl-2-isopropylcyclopentane	0.0091
1,2,3-trimethylbenzene	0.0113
2,5-dimethylnonane	0.0065
2,4,6-trimethyloctane	0.0046
2,6-dimethylnonane	0.0223
OTHER C9	0.0030
methyl propylcyclohexane	0.0103
isobutylcyclohexane	0.0086
butylcyclohexane	0.0073
pentylcyclopentane	0.0167
3,7-dimethylnonane	0.0083
5-methylindane	0.0089
1,3-dimethyl-5-ethylbenzene	0.0094
5-ethyl-2-methyloctane	0.0052
5-methyldecane	0.0188
4-methyldecane	0.0084
3-ethylnonane	0.0112
trans-decalin	0.0171
3-methyldecane	0.0141
ethyl propylcyclohexane	0.0043
ethyl propylcyclohexane	0.0036
1,3-dimethyl-2-ethylbenzene	0.0040
1,2-diethyl-1-methylcyclohexane	0.0083
1-ethyl-1,3-dimethylcyclohexane	0.0040
ethyl propylcyclohexane	0.0153
cis-decalin	0.0049
ethyl propylcyclohexane	0.0032
undecane	0.0630
2-methyldecalin	0.0133
ethyl propylcyclohexane	0.0070
1,2,4,5-tetramethylbenzene	0.0049
2-methyldecalin	0.0175
OTHER C12	0.0030
5-ethyl-3-methyloctane	0.0180
(2-methylbutyl)cyclohexane	0.0027
OTHER C12	0.0035
pentylcyclohexane	0.0097
1-cyclopentyl-2-methylpentane	0.0127
OTHER C12	0.0026
6-methylundecane	0.0120
4-methylundecane	0.0053
2-methylundecane	0.0094
3-methylundecane	0.0086
OTHER C12	0.0039
methyl pentylcyclohexane	0.0023
5,6-dimethylindane	0.0040
dodecane	0.0312
2,4-dimethylundecane	0.0019
6-methyldodecane	0.0066
hexylcyclohexane	0.0017
Total	1.0000
Fraction Identified	0.9820

SD48	
Compound	Fraction
3-methylpentane	0.0006
3,4-dimethylhexane	0.0010
1,1-dimethylcyclohexane	0.0009
Added ClBz	0.0000
ethylbenzene	0.0146
trans, trans-1,2,4-trimethylcyclohexane	0.0025
trans, trans-1,3,5-trimethylcyclohexane	0.0007
m-xylene	0.0360
p-xylene	0.0133
OTHER C9	0.0021
OTHER C9	0.0025
trans, cis-1,2,4-trimethylcyclohexane	0.0051
o-xylene	0.0174
cis, trans-1,2,4-trimethylcyclohexane	0.0032
1,2,3-trimethylcyclohexane	0.0028
cis-1-ethyl-3-methylcyclohexane	0.0025
cis-1-ethyl-3-methylcyclohexane	0.0106
trans-1-ethyl-3-methylcyclohexane	0.0060
OTHER C9	0.0021
nonane	0.0382
trans-1-ethyl-2-methylcyclohexane	0.0025
cis, trans-1,2,3-trimethylcyclohexane	0.0048
2,4-dimethyloctane	0.0168
cis-1-ethyl-4-methylcyclohexane	0.0040
OTHER C10	0.0009
isopropylbenzene	0.0021
3,4-dimethyloctane	0.0058
isopropylcyclohexane	0.0131
3,5-dimethyloctane	0.0065
2,5-dimethyloctane	0.0016
cis-1-ethyl-2-methylcyclohexane	0.0048
propylcyclohexane	0.0247
2,6-dimethyloctane	0.0262
3,3,5-trimethylheptane	0.0024
OTHER C10	0.0058
3,6-dimethyloctane	0.0059
1,1,2,3-tetramethylcyclohexane	0.0152
propylbenzene	0.0071
1,1,2,3-tetramethylcyclohexane	0.0032
1-ethyl-1,3-dimethylcyclohexane	0.0047
1-ethyl-3-methylbenzene	0.0155
1-ethyl-4-methylbenzene	0.0189
3-ethyl-4-methylheptane	0.0041
1,3,5-trimethylbenzene	0.0141
4-methylnonane	0.0174
2-methylnonane	0.0345
3-methylnonane	0.0072
1-ethyl-2-methylbenzene	0.0211
methyl isopropylcyclohexane	0.0026
1-methyl-3-isopropylcyclohexane	0.0120
1-methyl-3-isopropylcyclohexane	0.0075
2-ethyl-1,3-dimethylcyclohexane	0.0079
1-ethyl-1,2-dimethylcyclohexane	0.0044
1,2,4-trimethylbenzene	0.0437
cis-bicyclo[4.3.0]nonane	0.0146
methyl isopropylcyclohexane	0.0111
decane	0.0851
methyl propylcyclohexane	0.0076
methyl propylcyclohexane	0.0065
2,4-dimethylnonane	0.0029
2-ethyl-1,3-dimethylcyclohexane	0.0041
1,2,3-trimethylbenzene	0.0198
2,5-dimethylnonane	0.0105
2,6-dimethylnonane	0.0253
methyl propylcyclohexane	0.0025
indane	0.0069
methyl propylcyclohexane	0.0062
isobutylcyclohexane	0.0077
butylcyclohexane	0.0069
pentylcyclopentane	0.0147
3,7-dimethylnonane	0.0118
OTHER C11	0.0030
5-methylindane	0.0093
4-ethylnonane	0.0074
5-methyldecane	0.0051
4-methyldecane	0.0193
2-methyldecane	0.0105
5-isopropylnonane	0.0113
3-methyldecane	0.0134
trans-decalin	0.0141
1,1-dimethyl-2-propylcyclohexane	0.0030
1,3-dimethyl-2-ethylbenzene	0.0024
diethylcyclohexane	0.0034
diethylcyclohexane	0.0062
ethyl propylcyclohexane	0.0023
ethyl propylcyclohexane	0.0078
cis-decalin	0.0031
ethyl propylcyclohexane	0.0015
undecane	0.0372
OTHER C12	0.0026
ethyl propylcyclohexane	0.0042
2-methyldecalin	0.0036
2,4-dimethyldecane	0.0025
2,6-dimethyldecane	0.0075
2-methyldecalin	0.0017
3-methylnonane	0.0064
OTHER C12	0.0011
pentylcyclohexane	0.0038
hexylcyclopentane	0.0034
3-ethyldecane	0.0008
6-methylundecane	0.0025
5-methylundecane	0.0017
4-methylundecane	0.0027
2-methylundecane	0.0035
3-methylundecane	0.0035
dodecane	0.0114
2,6-dimethylundecane	0.0013
Total	1.0000
Fraction Identified	0.9799

SD49	
Compound	Fraction
3-methylpentane	0.0009
toluene	0.0022
4-methylheptane	0.0006
3,4-dimethylhexane	0.0014
cis-1,3-dimethylcyclohexane	0.0009
octane	0.0015
cis-1,4-dimethylcyclohexane	0.0007
2,6-dimethylheptane	0.0016
Added ClBz	0.0000
ethylcyclohexane	0.0011
2,5-dimethylheptane	0.0011
1,1,3-trimethylcyclohexane	0.0035
1,1,4-trimethylcyclohexane	0.0011
OTHER C9	0.0010
ethylbenzene	0.0120
trans, trans-1,3,5-trimethylcyclohexane	0.0050
2,3-dimethylheptane	0.0027
m-xylene	0.0330
p-xylene	0.0133
2-methyloctane	0.0061
3-methyloctane	0.0050
1,2,3-trimethylcyclohexane	0.0012
trans, cis-1,2,4-trimethylcyclohexane	0.0052
o-xylene	0.0206
cis, trans-1,2,4-trimethylcyclohexane	0.0026
1,2,3-trimethylcyclohexane	0.0035
trans-1-ethyl-3-methylcyclohexane	0.0022
cis-1-ethyl-3-methylcyclohexane	0.0089
trans-1-ethyl-4-methylcyclohexane	0.0049
cis, cis-1,2,4-trimethylcyclohexane	0.0031
nonane	0.0132
trans-1-ethyl-2-methylcyclohexane	0.0032
cis, trans-1,2,3-trimethylcyclohexane	0.0028
2,4-dimethyloctane	0.0117
cis-1-ethyl-4-methylcyclohexane	0.0039
OTHER C10	0.0006
isopropylbenzene	0.0022
3,4-dimethyloctane	0.0050
OTHER C10	0.0015
isopropylcyclohexane	0.0073
3,5-dimethyloctane	0.0070
2,5-dimethyloctane	0.0014
cis-1-ethyl-2-methylcyclohexane	0.0055
propylcyclohexane	0.0178
2,6-dimethyloctane	0.0160
3,3,5-trimethylheptane	0.0030
OTHER C10	0.0038
3,6-dimethyloctane	0.0054
1,1,2,3-tetramethylcyclohexane	0.0121
propylbenzene	0.0079
1,1,2,3-tetramethylcyclohexane	0.0032
1-ethyl-1,3-dimethylcyclohexane	0.0063
1-ethyl-3-methylbenzene	0.0164
1-ethyl-4-methylbenzene	0.0198
1,3,5-trimethylbenzene	0.0342
2-methylnonane	0.0314
3-methylnonane	0.0091
1-ethyl-2-methylbenzene	0.0244
3-ethyloctane	0.0029
1-methyl-3-isopropylcyclohexane	0.0130
1-methyl-3-isopropylcyclohexane	0.0134
methyl isopropylcyclohexane	0.0042
1,2,4-trimethylbenzene	0.0438
cis-bicyclo[4.3.0]nonane	0.0128
1-methyl-2-isopropylcyclohexane	0.0157
decane	0.0421
methyl propylcyclohexane	0.0062
methyl propylcyclohexane	0.0066
methyl propylcyclohexane	0.0114
2-ethyl-1,3-dimethylcyclohexane	0.0043
1,3-dimethyl-2-isopropylcyclopentane	0.0132
1,2,3-trimethylbenzene	0.0113
2,5-dimethylnonane	0.0123
2,6-dimethylnonane	0.0176
methyl propylcyclohexane	0.0043
methyl propylcyclohexane	0.0144
isobutylcyclohexane	0.0068
butylcyclohexane	0.0102
pentylcyclopentane	0.0143
3,7-dimethylnonane	0.0112
1,3-diethylbenzene	0.0049
OTHER C11	0.0091
1,3-dimethyl-5-ethylbenzene	0.0103
4-ethylnonane	0.0086
5-methyldecane	0.0207
4-methyldecane	0.0111
2-methyldecane	0.0121
trans-decalin	0.0034
5-isopropylnonane	0.0142
3-methyldecane	0.0182
1,1-dimethyl-2-propylcyclohexane	0.0049
ethyl propylcyclohexane	0.0067
1,2-diethyl-1-methylcyclohexane	0.0055
ethyl propylcyclohexane	0.0030
ethyl propylcyclohexane	0.0110
OTHER C11	0.0021
cis-decalin	0.0031
undecane	0.0357
ethyl propylcyclohexane	0.0107
2-methyldecalin	0.0054
ethyl propylcyclohexane	0.0054
2,6-dimethyldecane	0.0096
OTHER C12	0.0034
2-methyldecalin	0.0031
3,5-dimethylnonane	0.0124
OTHER C12	0.0020
(2-methylbutyl)cyclohexane	0.0033
pentylcyclohexane	0.0060
hexylcyclopentane	0.0059
OTHER C12	0.0016
6-methylundecane	0.0068
4-methylundecane	0.0030
2-methylundecane	0.0041
OTHER C12	0.0017
3-methylundecane	0.0025
naphthalene	0.0018
5,6-dimethylindane	0.0013
dodecane	0.0085
2,6-dimethylundecane	0.0016
Total	1.0000
Fraction Identified	0.9748

SD50	
Compound	Fraction
2-methylheptane	0.0010
3,4-dimethylhexane	0.0015
octane	0.0042
2-methyloctane	0.0029
Added ClBz	0.0000
ethylcyclohexane	0.0020
2,5-dimethylheptane	0.0011
1,1,3-trimethylcyclohexane	0.0048
ethylbenzene	0.0017
trans, trans-1,3,5-trimethylcyclohexane	0.0036
2,3-dimethylheptane	0.0028
m-xylene	0.0025
p-xylene	0.0011
4-methyloctane	0.0067
3-methyloctane	0.0065
trans, cis-1,2,4-trimethylcyclohexane	0.0010
1,2,3-trimethylcyclohexane	0.0046
o-xylene	0.0036
1,2,3-trimethylcyclohexane	0.0061
cis-1-ethyl-3-methylcyclohexane	0.0025
cis-1-ethyl-3-methylcyclohexane	0.0069
cis, cis-1,2,4-trimethylcyclohexane	0.0043
OTHER C9	0.0026
nonane	0.0342
trans-1-ethyl-2-methylcyclohexane	0.0031
cis, trans-1,2,3-trimethylcyclohexane	0.0028
2,4-dimethyloctane	0.0101
isopropylbenzene	0.0023
3,4-dimethyloctane	0.0043
isopropylcyclohexane	0.0117
3,5-dimethyloctane	0.0050
2,5-dimethyloctane	0.0012
cis-1-ethyl-2-methylcyclohexane	0.0036
propylcyclohexane	0.0166
2,6-dimethyloctane	0.0232
3,3,5-trimethylheptane	0.0026
butylcyclohexane	0.0056
3,6-dimethyloctane	0.0051
1,1,2,3-tetramethylcyclohexane	0.0136
propylbenzene	0.0052
1,1,2,3-tetramethylcyclohexane	0.0030
1-ethyl-1,3-dimethylcyclohexane	0.0044
1-ethyl-3-methylbenzene	0.0057
1-ethyl-4-methylbenzene	0.0134
OTHER C10	0.0026
1,3,5-trimethylbenzene	0.0058
4-methylnonane	0.0210
2-methylnonane	0.0371
3-methylnonane	0.0067
1-ethyl-2-methylbenzene	0.0187
3-ethyloctane	0.0044
1-methyl-3-isopropylcyclohexane	0.0122
1-methyl-3-isopropylcyclohexane	0.0090
2-ethyl-1,3-dimethylcyclohexane	0.0065
diethylcyclohexane	0.0044
1,2,4-trimethylbenzene	0.0292
diethylcyclohexane	0.0024
cis-bicyclo[4.3.0]nonane	0.0147
1-methyl-2-isopropylcyclohexane	0.0128
decane	0.1176
diethylcyclohexane	0.0057
methyl propylcyclohexane	0.0086
methyl propylcyclohexane	0.0077
OTHER C11	0.0021
2-ethyl-1,3-dimethylcyclohexane	0.0051
1,3-dimethyl-2-isopropylcyclopentane	0.0128
1,2,3-trimethylbenzene	0.0113
1-methyl-4-isopropylbenzene	0.0161
2,6-dimethylnonane	0.0409
methyl propylcyclohexane	0.0033
methyl propylcyclohexane	0.0136
isobutylcyclohexane	0.0099
1-methyl-2-isopropylbenzene	0.0096
pentylcyclopentane	0.0166
3,7-dimethylnonane	0.0155
1,3-diethylbenzene	0.0047
5-methylindane	0.0112
1,3-dimethyl-5-ethylbenzene	0.0121
4-ethylnonane	0.0049
5-methyldecane	0.0210
4-methyldecane	0.0083
2-methyldecane	0.0122
5-isopropylnonane	0.0107
3-methyldecane	0.0135
ethyl propylcyclohexane	0.0031
1,1-dimethyl-2-propylcyclohexane	0.0021
1-methylindane	0.0023
ethyl propylcyclohexane	0.0043
1,3-dimethyl-2-ethylbenzene	0.0037
ethyl propylcyclohexane	0.0030
methyl butylcyclohexane	0.0087
OTHER C12	0.0011
cis-decalin	0.0016
undecane	0.0488
1-ethyl-4-isopropylbenzene	0.0028
ethyl propylcyclohexane	0.0047
2-methyldecalin	0.0032
2,4-dimethyldecane	0.0026
1,2,4,5-tetramethylbenzene	0.0027
2,6-dimethyldecane	0.0103
3-methylnonane	0.0077
2,7-dimethyldecane	0.0014
OTHER C12	0.0013
(2-methylbutyl)cyclohexane	0.0034
pentylcyclohexane	0.0049
hexylcyclopentane	0.0041
4-ethyldecane	0.0016
1,2,3,4-tetramethylbenzene	0.0085
OTHER C12	0.0011
tetralin	0.0018
2-methylundecane	0.0066
3-methylundecane	0.0033
naphthalene	0.0031
methyl pentylcyclohexane	0.0011
dodecane	0.0100
2,6-dimethylundecane	0.0020
Total	1.0000
Fraction Identified	0.9891

SD51	
Compound	Fraction
ethanol	0.0162
methyl ethyl ketone	0.0023
Added Benzene	0.0000
methylcyclohexane	0.0006
toluene	0.0018
2-methyloctane	0.0006
Added ClBz	0.0000
ethylcyclohexane	0.0005
1,1,3-trimethylcyclohexane	0.0020
ethylbenzene	0.0012
trans, trans-1,3,5-trimethylcyclohexane	0.0052
2,3-dimethylheptane	0.0020
m-xylene	0.0019
p-xylene	0.0009
4-methyloctane	0.0045
3-methyloctane	0.0044
1,2,3-trimethylcyclohexane	0.0063
o-xylene	0.0052
1,2,3-trimethylcyclohexane	0.0064
cis-1-ethyl-3-methylcyclohexane	0.0019
cis-1-ethyl-4-methylcyclohexane	0.0111
cis, cis-1,2,4-trimethylcyclohexane	0.0060
OTHER C9	0.0011
OTHER C9	0.0007
nonane	0.0319
trans-1-ethyl-2-methylcyclohexane	0.0020
trans-1-ethyl-3-methylcyclohexane	0.0046
2,4-dimethyloctane	0.0163
isopropylbenzene	0.0040
OTHER C10	0.0011
3,4-dimethyloctane	0.0062
isopropylcyclohexane	0.0123
3,5-dimethyloctane	0.0071
2,5-dimethyloctane	0.0018
cis-1-ethyl-2-methylcyclohexane	0.0051
propylcyclohexane	0.0253
2,6-dimethyloctane	0.0254
3,3,5-trimethylheptane	0.0026
butylcyclohexane	0.0062
3,6-dimethyloctane	0.0064
1,1,2,3-tetramethylcyclohexane	0.0171
propylbenzene	0.0045
1,1,2,3-tetramethylcyclohexane	0.0038
1-ethyl-1,3-dimethylcyclohexane	0.0052
1-ethyl-3-methylbenzene	0.0030
1-ethyl-4-methylbenzene	0.0179
1,3,5-trimethylbenzene	0.0128
4-methylnonane	0.0214
2-methylnonane	0.0382
3-methylnonane	0.0086
1-ethyl-2-methylbenzene	0.0198
1-methyl-4-isopropylcyclohexane	0.0040
1-methyl-3-isopropylcyclohexane	0.0138
1-methyl-4-isopropylcyclohexane	0.0084
2-ethyl-1,3-dimethylcyclohexane	0.0084
trans-1,2-dimethylcyclohexane	0.0052
1,2,4-trimethylbenzene	0.0273
cis-bicyclo[4.3.0]nonane	0.0156
1-methyl-2-isopropylcyclohexane	0.0066
diethylcyclohexane	0.0060
decane	0.1048
diethylcyclohexane	0.0090
diethylcyclohexane	0.0078
diethylcyclohexane	0.0034
1-methyl-3-isopropylbenzene	0.0044
1,3-dimethyl-2-isopropylcyclopentane	0.0139
1,2,3-trimethylbenzene	0.0054
2,5-dimethylnonane	0.0117
2,6-dimethylnonane	0.0282
methyl propylcyclohexane	0.0030
methyl propylcyclohexane	0.0140
isobutylcyclohexane	0.0087
1-methyl-2-isopropylbenzene	0.0084
pentylcyclopentane	0.0176
3,7-dimethylnonane	0.0124
1,3-diethylbenzene	0.0035
5-methylindane	0.0086
1,3-dimethyl-5-ethylbenzene	0.0080
4-ethylnonane	0.0062
3-ethylnonane	0.0040
5-methyldecane	0.0167
4-methyldecane	0.0119
2-methyldecane	0.0121
OTHER C11	0.0019
5-isopropylnonane	0.0140
3-methyldecane	0.0157
1,1-dimethyl-2-propylcyclohexane	0.0032
1-methylindane	0.0026
OTHER C11	0.0032
1,3-dimethyl-2-ethylbenzene	0.0049
ethyl propylcyclohexane	0.0025
methyl butylcyclohexane	0.0103
cis-decalin	0.0022
methyl butylcyclohexane	0.0019
undecane	0.0468
1-ethyl-4-isopropylbenzene	0.0077
2-methyldecalin	0.0068
1,2,4,5-tetramethylbenzene	0.0029
3,6-dimethyldecane	0.0066
2-methyldecalin	0.0023
2,6-dimethyldecane	0.0020
3,7-dimethyldecane	0.0072
4,5-dimethyldecane	0.0013
pentylcyclohexane	0.0050
4-methylindane	0.0038
4-ethyldecane	0.0010
6-methylundecane	0.0029
5-methylundecane	0.0021
tetralin	0.0032
2-methylundecane	0.0039
3-methylundecane	0.0041
dodecane	0.0135
2,4-dimethylundecane	0.0006
2,6-dimethylundecane	0.0016
Total	1.0000
Fraction Identified	0.9921

SD52	
Compound	Fraction
trans-1,4-dimethylcyclohexane	0.0008
octane	0.0021
2-methyloctane	0.0013
Added ClBz	0.0000
ethylcyclohexane	0.0013
1,1,3-trimethylcyclohexane	0.0016
ethylbenzene	0.0037
trans, trans-1,3,5-trimethylcyclohexane	0.0075
2,3-dimethylheptane	0.0019
m-xylene	0.0080
p-xylene	0.0032
4-methyloctane	0.0027
3-methyloctane	0.0029
1,2,3-trimethylcyclohexane	0.0061
o-xylene	0.0087
cis, trans-1,2,4-trimethylcyclohexane	0.0034
1,2,3-trimethylcyclohexane	0.0019
cis-1-ethyl-3-methylcyclohexane	0.0013
cis-1-ethyl-3-methylcyclohexane	0.0089
cis, cis-1,2,4-trimethylcyclohexane	0.0045
OTHER C9	0.0009
nonane	0.0234
trans-1-ethyl-2-methylcyclohexane	0.0022
trans-1-ethyl-4-methylcyclohexane	0.0033
2,4-dimethyloctane	0.0125
isopropylbenzene	0.0031
OTHER C10	0.0007
2,3,5-trimethylheptane	0.0010
3,4-dimethyloctane	0.0043
isopropylcyclohexane	0.0093
3,5-dimethyloctane	0.0056
2,5-dimethyloctane	0.0012
cis-1-ethyl-2-methylcyclohexane	0.0044
propylcyclohexane	0.0197
2,6-dimethyloctane	0.0219
3,3,5-trimethylheptane	0.0026
4,5-dimethyloctane	0.0041
3,6-dimethyloctane	0.0046
1,1,2,3-tetramethylcyclohexane	0.0181
propylbenzene	0.0064
1,1,2,3-tetramethylcyclohexane	0.0036
1-ethyl-1,3-dimethylcyclohexane	0.0053
1-ethyl-3-methylbenzene	0.0086
1-ethyl-4-methylbenzene	0.0184
1,3,5-trimethylbenzene	0.0103
4-methylnonane	0.0218
2-methylnonane	0.0337
3-methylnonane	0.0083
1-ethyl-2-methylbenzene	0.0201
diethylcyclohexane	0.0037
1-methyl-3-isopropylcyclohexane	0.0121
1-methyl-3-isopropylcyclohexane	0.0080
2-ethyl-1,3-dimethylcyclohexane	0.0061
diethylcyclohexane	0.0042
1,2,4-trimethylbenzene	0.0389
1-methyl-2-isopropylcyclohexane	0.0137
diethylcyclohexane	0.0114
decane	0.0839
methyl propylcyclohexane	0.0058
methyl propylcyclohexane	0.0078
methyl propylcyclohexane	0.0104
2-ethyl-1,3-dimethylcyclohexane	0.0025
1,3-dimethyl-2-isopropylcyclopentane	0.0127
1,2,3-trimethylbenzene	0.0117
2,4,6-trimethyloctane	0.0114
2,6-dimethylnonane	0.0263
methyl propylcyclohexane	0.0028
methyl propylcyclohexane	0.0144
4,5-dimethylnonane	0.0076
1-methyl-2-isopropylbenzene	0.0096
pentylcyclopentane	0.0174
3,7-dimethylnonane	0.0137
1,3-diethylbenzene	0.0040
5-methylindane	0.0110
1,3-dimethyl-5-ethylbenzene	0.0110
4-ethylnonane	0.0066
5-methyldecane	0.0215
4-methyldecane	0.0116
2-methyldecane	0.0155
OTHER C11	0.0019
1,2-dimethyl-4-ethylbenzene	0.0123
1,4-dimethyl-2-ethylbenzene	0.0177
1,1-dimethyl-2-propylcyclohexane	0.0035
1,3-dimethyl-2-ethylbenzene	0.0079
OTHER C11	0.0063
ethyl propylcyclohexane	0.0032
methyl butylcyclohexane	0.0123
cis-decalin	0.0054
ethyl propylcyclohexane	0.0023
undecane	0.0609
ethyl propylcyclohexane	0.0049
1-ethyl-4-isopropylbenzene	0.0070
2-methyldecalin	0.0078
1,2,4,5-tetramethylbenzene	0.0047
2,5-dimethyldecane	0.0133
1,2,3,5-tetramethylbenzene	0.0026
2-methyldecalin	0.0046
3,5-dimethyldecane	0.0114
2,6-dimethyldecane	0.0025
2,7-dimethyldecane	0.0030
pentylcyclohexane	0.0073
hexylcyclopentane	0.0039
4-ethyldecane	0.0016
1,2,3,4-tetramethylbenzene	0.0071
tetralin	0.0024
2-methylundecane	0.0035
3-methylundecane	0.0021
dodecane	0.0073
2,6-dimethylundecane	0.0008
Total	1.0000
Fraction Identified	0.9901

SD53	
Compound	Fraction
toluene	0.0031
octane	0.0015
2,6-dimethylheptane	0.0011
ethylcyclohexane	0.0014
cis, cis-1,3,5-trimethylcyclohexane	0.0011
1,1,3-trimethylcyclohexane	0.0013
ethylbenzene	0.0026
trans, trans-1,2,4-trimethylcyclohexane	0.0030
trans, trans-1,3,5-trimethylcyclohexane	0.0013
m-xylene	0.0060
p-xylene	0.0016
2-methyloctane	0.0026
trans, cis-1,2,4-trimethylcyclohexane	0.0027
cis-1-ethyl-2-methylcyclohexane	0.0025
o-xylene	0.0055
1,2,3-trimethylcyclohexane	0.0030
cis-1-ethyl-3-methylcyclohexane	0.0033
cis, cis-1,2,4-trimethylcyclohexane	0.0014
nonane	0.0137
trans-1-ethyl-2-methylcyclohexane	0.0008
trans-1-ethyl-3-methylcyclohexane	0.0011
2,4-dimethyloctane	0.0046
cis-1-ethyl-4-methylcyclohexane	0.0009
isopropylbenzene	0.0013
isopropylcyclohexane	0.0034
3,5-dimethyloctane	0.0013
OTHER C10	0.0010
propylcyclohexane	0.0063
2,6-dimethyloctane	0.0075
1,1,2,3-tetramethylcyclohexane	0.0061
propylbenzene	0.0023
3-ethyl-2-methylheptane	0.0009
1,1,2,3-tetramethylcyclohexane	0.0013
1-ethyl-3-methylbenzene	0.0030
1-ethyl-4-methylbenzene	0.0050
1,3,5-trimethylbenzene	0.0095
2,3-dimethyloctane	0.0054
2-methylnonane	0.0044
3-methylnonane	0.0021
1-ethyl-2-methylbenzene	0.0055
1-methyl-4-isopropylcyclohexane	0.0010
1-methyl-3-isopropylcyclohexane	0.0032
1-methyl-3-isopropylcyclohexane	0.0025
2-ethyl-1,3-dimethylcyclohexane	0.0018
1,2,4-trimethylbenzene	0.0129
cis-bicyclo[4.3.0]nonane	0.0041
1,1,3,4-tetramethylcyclohexane	0.0031
decane	0.0306
methyl propylcyclohexane	0.0019
methyl propylcyclohexane	0.0025
methyl propylcyclohexane	0.0031
2-ethyl-1,3-dimethylcyclohexane	0.0019
1,2,3-trimethylbenzene	0.0052
2,5-dimethylnonane	0.0032
2,6-dimethylnonane	0.0092
methyl propylcyclohexane	0.0035
isobutylcyclohexane	0.0024
butylcyclohexane	0.0026
pentylcyclopentane	0.0068
3,7-dimethylnonane	0.0067
OTHER C11	0.0017
5-methylindane	0.0061
2,3-dimethylnonane	0.0056
4-ethylnonane	0.0040
5-methyldecane	0.0211
4-methyldecane	0.0108
2-methyldecane	0.0159
OTHER C11	0.0027
trans-decalin	0.0179
3-methyldecane	0.0257
1,1-dimethyl-2-propylcyclohexane	0.0061
1,3-dimethyl-2-ethylbenzene	0.0059
diethylcyclohexane	0.0072
diethylcyclohexane	0.0157
ethyl propylcyclohexane	0.0076
cis-decalin	0.0302
ethyl propylcyclohexane	0.0120
ethyl propylcyclohexane	0.0057
undecane	0.1626
ethyl propylcyclohexane	0.0121
6-ethyl-2-methyloctane	0.0215
2-methyldecalin	0.0261
2,4-dimethyldecane	0.0091
3,6-dimethyldecane	0.0284
2,6-dimethyldecane	0.0081
2-methyldecalin	0.0076
3,6-dimethyldecane	0.0365
2,7-dimethyldecane	0.0039
4,5-dimethyldecane	0.0046
OTHER C12	0.0018
butyl methylcyclohexane	0.0047
pentylcyclohexane	0.0265
4-methylindane	0.0150
1,2,3,4-tetramethylbenzene	0.0033
6-methylundecane	0.0198
4-methylundecane	0.0095
tetralin	0.0012
2-methylundecane	0.0136
OTHER C12	0.0009
3-methylundecane	0.0078
OTHER C12	0.0041
OTHER C12	0.0022
naphthalene	0.0049
methyl pentylcyclohexane	0.0045
5,6-dimethylindane	0.0074
dodecane	0.0502
2,6-dimethyldodecane	0.0051
1,1,5-trimethylindane	0.0019
2,6-dimethylundecane	0.0091
OTHER C13	0.0019
2,4-dimethylundecane	0.0029
2-butyl-1,1,3-trimethylcyclohexane	0.0026
OTHER C13	0.0012
OTHER C13	0.0015
6-methyldodecane	0.0030
hexylcyclohexane	0.0049
4-ethylundecane	0.0013
5-methyldodecane	0.0019
4-methyldodecane	0.0021
3-ethylundecane	0.0026
2,10-dimethylundecane	0.0018
3-methyldodecane	0.0034
OTHER C13	0.0048
Added C13	0.0000
OTHER C14	0.0034
OTHER C14	0.0015
OTHER C14	0.0028
Total	1.0000
Fraction Identified	0.9685

SD54	
Compound	Fraction
toluene	0.0026
trans-1,4-dimethylcyclohexane	0.0005
octane	0.0012
2,6-dimethylheptane	0.0009
cis, cis-1,3,5-trimethylcyclohexane	0.0010
ethylcyclohexane	0.0009
1,1,4-trimethylcyclohexane	0.0011
ethylbenzene	0.0020
trans, trans-1,3,5-trimethylcyclohexane	0.0024
2,3-dimethylheptane	0.0010
m-xylene	0.0049
p-xylene	0.0012
4-methyloctane	0.0021
3-methyloctane	0.0022
1,2,3-trimethylcyclohexane	0.0020
o-xylene	0.0045
1,2,3-trimethylcyclohexane	0.0025
cis-1-ethyl-3-methylcyclohexane	0.0027
cis, cis-1,2,4-trimethylcyclohexane	0.0013
nonane	0.0113
trans-1-ethyl-2-methylcyclohexane	0.0007
cis, trans-1,2,3-trimethylcyclohexane	0.0010
2,4-dimethyloctane	0.0039
isopropylbenzene	0.0008
3,4-dimethyloctane	0.0011
isopropylcyclohexane	0.0032
3,5-dimethyloctane	0.0012
cis-1-ethyl-2-methylcyclohexane	0.0009
propylcyclohexane	0.0051
2,6-dimethyloctane	0.0062
2,7-dimethyloctane	0.0011
3,6-dimethyloctane	0.0050
propylbenzene	0.0019
1,1,2,3-tetramethylcyclohexane	0.0008
1-ethyl-1,3-dimethylcyclohexane	0.0011
1-ethyl-3-methylbenzene	0.0025
1-ethyl-4-methylbenzene	0.0042
1,3,5-trimethylbenzene	0.0079
4-methylnonane	0.0044
2-methylnonane	0.0036
3-methylnonane	0.0017
1-ethyl-2-methylbenzene	0.0046
OTHER C10	0.0008
1-methyl-3-isopropylcyclohexane	0.0027
1-methyl-3-isopropylcyclohexane	0.0021
2-ethyl-1,3-dimethylcyclohexane	0.0016
OTHER C10	0.0009
1,2,4-trimethylbenzene	0.0107
cis-bicyclo[4.3.0]nonane	0.0034
1-methyl-2-isopropylcyclohexane	0.0026
decane	0.0253
methyl propylcyclohexane	0.0015
methyl propylcyclohexane	0.0020
methyl propylcyclohexane	0.0025
2-ethyl-1,3-dimethylcyclohexane	0.0005
1,3-dimethyl-2-isopropylcyclopentane	0.0017
1,2,3-trimethylbenzene	0.0045
1-methyl-4-isopropylbenzene	0.0028
2,6-dimethylnonane	0.0081
2,7-dimethylnonane	0.0021
methyl propylcyclohexane	0.0016
4,5-dimethylnonane	0.0027
1-methyl-2-isopropylbenzene	0.0026
pentylcyclopentane	0.0062
3,7-dimethylnonane	0.0062
1,3-diethylbenzene	0.0019
5-methylindane	0.0061
1,3-dimethyl-5-ethylbenzene	0.0060
4-ethylnonane	0.0041
5-methyldecane	0.0199
4-methyldecane	0.0101
cis-decalin	0.0149
2-methyldecane	0.0028
5-isopropylnonane	0.0166
3-methyldecane	0.0244
1,2-dimethyl-4-ethylbenzene	0.0065
1,3-dimethyl-2-ethylbenzene	0.0061
ethyl propylcyclohexane	0.0077
1,4-dimethyl-2-ethylbenzene	0.0171
ethyl propylcyclohexane	0.0080
methyl butylcyclohexane	0.0278
cis-decalin	0.0122
ethyl propylcyclohexane	0.0059
undecane	0.1385
ethyl propylcyclohexane	0.0124
2-methyldecalin	0.0202
2-methyl-6-ethyloctane	0.0274
2,4-dimethyldecane	0.0104
3,6-dimethyldecane	0.0288
2-methyldecalin	0.0095
3,5-dimethyldecane	0.0092
3,7-dimethyldecane	0.0365
2,7-dimethyldecane	0.0065
4,5-dimethyldecane	0.0067
OTHER C12	0.0036
butyl methylcyclohexane	0.0075
pentylcyclohexane	0.0271
hexylcyclopentane	0.0174
5-ethyldecane	0.0065
5-methylundecane	0.0231
4-methylundecane	0.0134
tetralin	0.0029
2-methylundecane	0.0156
OTHER C12	0.0054
3-methylundecane	0.0175
OTHER C12	0.0073
OTHER C12	0.0044
naphthalene	0.0095
methyl pentylcyclohexane	0.0060
5,6-dimethylindane	0.0085
dodecane	0.0419
OTHER C13	0.0061
OTHER C13	0.0022
2,6-dimethylundecane	0.0076
2,5-dimethylundecane	0.0019
3,6-dimethylundecane	0.0028
2-butyl-1,1,3-trimethylcyclohexane	0.0022
OTHER C13	0.0011
OTHER C13	0.0013
pentamethylbenzene	0.0020
(4-methylpentyl)cyclohexane	0.0024
hexylcyclohexane	0.0038
6-methyldodecane	0.0010
4-ethylundecane	0.0015
4-methyldodecane	0.0015
2,10-dimethylundecane	0.0018
OTHER C13	0.0013
3-methyldodecane	0.0024
4,5-dimethylundecane	0.0033
tridecane	0.0115
2-methylnaphthalene	0.0025
OTHER C13	0.0010
2-ethyltetralin	0.0019
5-methyltridecane	0.0022
2-methyltridecane	0.0007
2,7,10-trimethylundecane	0.0039
OTHER C14	0.0023
Total	1.0000
Fraction Identified	0.9623

SD55	
Compound	Fraction
methylcyclohexane	0.0006
toluene	0.0006
2-methylheptane	0.0006
cis-1,3-dimethylcyclohexane	0.0015
trans-1,4-dimethylcyclohexane	0.0005
octane	0.0021
cis-1,4-dimethylcyclohexane	0.0008
2,6-dimethylheptane	0.0014
2,7-dimethylheptane	0.0009
ethylcyclohexane	0.0012
1,1,3-trimethylcyclohexane	0.0026
OTHER C9	0.0007
OTHER C9	0.0006
ethylbenzene	0.0037
trans, trans-1,2,4-trimethylcyclohexane	0.0028
2,3-dimethylheptane	0.0012
m-xylene	0.0094
p-xylene	0.0033
4-methyloctane	0.0012
OTHER C9	0.0008
3-methyloctane	0.0012
1,2,3-trimethylcyclohexane	0.0023
o-xylene	0.0163
cis, trans-1,2,4-trimethylcyclohexane	0.0128
1-methyl-2-propylcyclopentane	0.0009
cis-1-ethyl-3-methylcyclohexane	0.0032
trans-1-ethyl-3-methylcyclohexane	0.0018
nonane	0.0037
trans-1-ethyl-2-methylcyclohexane	0.0014
cis, trans-1,2,3-trimethylcyclohexane	0.0009
trans-1-ethyl-4-methylcyclohexane	0.0035
cis-1-ethyl-4-methylcyclohexane	0.0009
isopropylbenzene	0.0192
2,3,5-trimethylheptane	0.0009
2,4-dimethyloctane	0.0006
isopropylcyclohexane	0.0029
2,5-dimethyloctane	0.0012
cis-1-ethyl-2-methylcyclohexane	0.0014
propylcyclohexane	0.0046
2,6-dimethyloctane	0.0043
butylcyclopentane	0.0013
1,1,2,3-tetramethylcyclohexane	0.0036
propylbenzene	0.0501
1-ethyl-1,3-dimethylcyclohexane	0.0016
1-ethyl-3-methylbenzene	0.1557
1-ethyl-4-methylbenzene	0.0716
1,3,5-trimethylbenzene	0.0841
2-methylnonane	0.0029
OTHER C10	0.0042
3-ethyloctane	0.0025
1-ethyl-2-methylbenzene	0.0621
3-methylnonane	0.0009
1-methyl-3-isopropylcyclohexane	0.0029
1-methyl-3-isopropylcyclohexane	0.0034
2-ethyl-1,3-dimethylcyclohexane	0.0016
1,2,4-trimethylbenzene	0.1466
1-methyl-2-isopropylcyclohexane	0.0036
diethylcyclohexane	0.0041
decane	0.0105
methyl propylcyclohexane	0.0018
sec-butylbenzene	0.0026
diethylcyclohexane	0.0036
2-ethyl-1,3-dimethylcyclohexane	0.0013
1-methyl-3-isopropylbenzene	0.0034
1,2,3-trimethylbenzene	0.0320
2,5-dimethylnonane	0.0024
2,6-dimethylnonane	0.0041
methyl propylcyclohexane	0.0023
indane	0.0095
isobutylcyclohexane	0.0016
butylcyclohexane	0.0021
pentylcyclopentane	0.0047
3,7-dimethylnonane	0.0028
1,3-diethylbenzene	0.0042
1-methyl-3-propylbenzene	0.0087
1,3-dimethyl-5-ethylbenzene	0.0171
5-methyldecane	0.0046
4-methyldecane	0.0016
1-methyl-2-propylbenzene	0.0033
trans-decalin	0.0014
3-methyldecane	0.0058
1,4-dimethyl-2-ethylbenzene	0.0069
1,3-dimethyl-4-ethylbenzene	0.0033
1,1-dimethyl-2-propylcyclohexane	0.0018
1,2-dimethyl-4-ethylbenzene	0.0070
1,3-dimethyl-2-ethylbenzene	0.0015
ethyl propylcyclohexane	0.0009
cis-decalin	0.0065
ethyl propylcyclohexane	0.0007
OTHER C11	0.0008
ethyl propylcyclohexane	0.0018
undecane	0.0074
2-methyldecalin	0.0039
OTHER C12	0.0017
1,2,4,5-tetramethylbenzene	0.0020
1,2,3,5-tetramethylbenzene	0.0042
2-methyldecalin	0.0017
1,3-dimethyl-4-isopropylbenzene	0.0108
(2-methylbutyl)cyclohexane	0.0012
5-methylindane	0.0021
hexylcyclopentane	0.0015
pentylcyclohexane	0.0064
4-methylindane	0.0055
1,2,3,4-tetramethylbenzene	0.0022
4-ethyldecane	0.0054
5-methylundecane	0.0016
4-methylundecane	0.0018
OTHER C12	0.0011
2-methylundecane	0.0033
3-methylundecane	0.0058
OTHER C12	0.0017
methyl pentylcyclohexane	0.0013
naphthalene	0.0049
5,6-dimethylindane	0.0049
dodecane	0.0058
OTHER C13	0.0047
1,3,5-triethylbenzene	0.0025
1,1,5-trimethylindane	0.0030
2,6-dimethylundecane	0.0025
3,6-dimethylundecane	0.0014
2,7-dimethylundecane	0.0025
OTHER C13	0.0005
hexylcyclohexane	0.0011
2,9-dimethylundecane	0.0026
4,7-dimethylindane	0.0011
2,10-dimethylundecane	0.0007
OTHER C13	0.0016
tridecane	0.0025
Total	1.0000
Fraction Identified	0.9868

Appendix E

COMPOSITE GROUP SPECIES PROFILES

Group 1w: Water-Based Flats/ Low-Gloss/Medium Gloss	
Compound	**Fraction**
Texanol	0.3522
propylene glycol	0.3331
ethylene glycol	0.1722
diethylene glycol butyl ether	0.0601
diethylene glycol methyl ether	0.0270
2-butoxyethanol	0.0146
diethylene glycol	0.0098
sec-butyl alcohol	0.0093
hexylene glycol	0.0070
1-amino-2-methyl-2-propanol	0.0039
1-butoxy-2-propanol	0.0021
isopropyl alcohol	0.0021
dipropylene glycol methyl ether	0.0019
unknown C9	0.0019
unknown C12	0.0015
unknown C8	0.0012
Total	***1.0000***

Group 2w: Water-Based Clear Wood Finishes	
Compound	**Fraction**
2-butoxyethanol	0.2675
N-methylpyrrolidone	0.2421
2-methoxy-1-propanol	0.1429
isopropyl alcohol	0.1357
dipropylene glycol methyl ether	0.0595
propylene glycol	0.0590
Texanol	0.0328
dibutyl phthalate	0.0232
methyl amyl ketone	0.0165
1-butoxy-2-propanol	0.0137
sec-butyl alcohol	0.0071
Total	***1.0000***

Group 6-w: Water-Based Semi-transparent Stains	
Compound	**Fraction**
propylene glycol	0.6044
2-butoxyethanol	0.0878
diethylene glycol butyl ether	0.0857
dipropylene glycol monobutyl ether	0.0684
1-propoxy-2-propanol	0.0657
isopropyl alcohol	0.0591
diethylene glycol ethyl ether	0.0180
N-methylpyrrolidone	0.0108
Total	***1.0000***

Group 7w: Water-based Traffic Paints	
Compound	**Fraction**
methanol	0.3720
diethylene glycol butyl ether	0.2353
Texanol	0.1497
ethanol	0.1088
ethylene glycol	0.0969
propylene glycol	0.0217
isopropyl alcohol	0.0085
2-butoxyethanol	0.0072
Total	***1.0000***

Group 2s: Solvent-based Clear Wood Finishes			
Compound	Fraction	cum frac	# of cmpds.
butyl acetate	0.1424	0.1424	1
m-xylene	0.0560	0.1984	2
methyl ethyl ketone	0.0508	0.2492	3
toluene	0.0402	0.2894	4
acetone	0.0396	0.3289	5
2-butoxyethanol	0.0367	0.3657	6
isobutyl isobutyrate	0.0360	0.4017	7
o-xylene	0.0314	0.4331	8
2-propanol	0.0312	0.4643	9
decane	0.0307	0.4951	10
methyl amyl ketone	0.0301	0.5252	11
butyl alcohol	0.0257	0.5509	12
p-xylene	0.0209	0.5718	13
ethylbenzene	0.0200	0.5918	14
ethanol	0.0174	0.6092	15
ethyl-3-ethoxypropionate	0.0160	0.6251	16
1-acetoxy-2-butoxyethane	0.0133	0.6384	17
4-methylnonane	0.0130	0.6514	18
diethylcyclohexane	0.0117	0.6631	19
nonane	0.0116	0.6747	20
methylcyclohexane	0.0106	0.6853	21
undecane	0.0095	0.6949	22
2,6-dimethylnonane	0.0087	0.7035	23
methyl propylcyclohexane	0.0087	0.7122	24
propylcyclohexane	0.0086	0.7208	25
heptane	0.0085	0.7294	26
2,6-dimethyloctane	0.0083	0.7377	27
1-methyl-2-isopropylcyclohexane	0.0075	0.7452	28
OTHER C11	0.0072	0.7523	29
1,2,4-trimethylbenzene	0.0070	0.7593	30
1,1,3-trimethylcyclopentane	0.0065	0.7659	31
1,3,5-trimethylbenzene	0.0060	0.7719	32
1-ethyl-4-methylbenzene	0.0059	0.7779	33
1,2-dimethylcyclopentane	0.0058	0.7837	34
trans-1-ethyl-4-methylcyclohexane	0.0057	0.7894	35
1,2-dimethyl-3-ethylcyclohexane	0.0051	0.7946	36
3-methylnonane	0.0050	0.7996	37
5-methyldecane	0.0050	0.8046	38
butylcyclohexane	0.0046	0.8092	39
octane	0.0045	0.8137	40
3,5-dimethyloctane	0.0045	0.8182	41
1,2,3-trimethylbenzene	0.0043	0.8225	42
cis-1-ethyl-3-methylcyclohexane	0.0042	0.8267	43
1,4-dimethyl-2-ethylbenzene	0.0041	0.8307	44
1-methyl-3-isopropylcyclohexane	0.0040	0.8348	45
3-ethyloctane	0.0039	0.8387	46
1,2,3-trimethylcyclopentane	0.0039	0.8425	47
OTHER C10	0.0038	0.8463	48
5-methylnonane	0.0037	0.8500	49
3,7-dimethylnonane	0.0034	0.8534	50
isobutylcyclohexane	0.0034	0.8569	51
cis-1,3-dimethylcyclohexane	0.0034	0.8603	52
2,3-dimethylnonane	0.0033	0.8636	53
ethyl propylcyclohexane	0.0033	0.8669	54
cis-1,3-dimethylcyclopentane	0.0031	0.8699	55
3,6-dimethyloctane	0.0030	0.8730	56
trans-1,3-dimethylcyclopentane	0.0030	0.8760	57
4-methyldecane	0.0030	0.8790	58
pentylcyclopentane	0.0029	0.8819	59
1,2,4-trimethylcyclopentane	0.0029	0.8848	60
3-methylhexane	0.0029	0.8876	61
trans, trans-1,3,5-trimethylcyclohexane	0.0027	0.8904	62
dodecane	0.0027	0.8931	63
2-methyldecalin	0.0026	0.8957	64
2-methyldecane	0.0026	0.8984	65
cis-decalin	0.0026	0.9009	66
2,5-dimethylnonane	0.0026	0.9035	67
5-methylindane	0.0025	0.9060	68
3-methyloctane	0.0024	0.9084	69
trans-1-ethyl-3-methylcyclohexane	0.0023	0.9106	70
1,1,3-trimethylcyclohexane	0.0023	0.9129	71
2,5-dimethyloctane	0.0022	0.9151	72
3,7-dimethyldecane	0.0022	0.9173	73
1,2,3-trimethylcyclohexane	0.0022	0.9195	74
2-methylheptane	0.0021	0.9216	75
trans, trans-1,2,4-trimethylcyclohexane	0.0021	0.9237	76
ethylcyclohexane	0.0020	0.9257	77
1,3-dimethyl-5-ethylbenzene	0.0020	0.9277	78
2,4,6-trimethylheptane	0.0019	0.9296	79
2,4-dimethylnonane	0.0019	0.9315	80
trans-decalin	0.0019	0.9334	81
1,2,3,5-tetramethylbenzene	0.0018	0.9352	82
2,4-dimethylhexane	0.0018	0.9370	83
5-ethyl-2-methyloctane	0.0018	0.9388	84
cis-1,2-dimethylcyclohexane	0.0018	0.9406	85
methyl butylcyclopentane	0.0018	0.9423	86
cis, trans-1,2,3-trimethylcyclohexane	0.0017	0.9441	87
2-methylhexane	0.0017	0.9458	88
cis, trans-1,2,4-trimethylcyclohexane	0.0017	0.9475	89
propylbenzene	0.0016	0.9491	90
2,3-dimethyloctane	0.0016	0.9506	91
4-methyloctane	0.0015	0.9521	92
2,7-dimethyloctane	0.0015	0.9536	93
2,5-dimethylhexane	0.0014	0.9550	94
cis-1-ethyl-4-methylcyclohexane	0.0013	0.9563	95
3-ethyl-4-methylheptane	0.0013	0.9576	96
trans, cis-1,2,4-trimethylcyclohexane	0.0013	0.9590	97
tetralin	0.0013	0.9603	98
sec butylcyclopentane	0.0013	0.9616	99
1-ethyl-3-methylbenzene	0.0013	0.9628	100
2-methyloctane	0.0013	0.9641	101
4-ethyldecane	0.0012	0.9653	102
cyclohexane	0.0012	0.9666	103
trans-1,3-dimethylcyclohexane	0.0012	0.9678	104
3-methylheptane	0.0012	0.9690	105
methanol	0.0012	0.9701	106
trans-1,4-dimethylcyclohexane	0.0011	0.9712	107
2-methylundecane	0.0011	0.9724	108
isopropylcyclohexane	0.0011	0.9735	109
pentylcyclohexane	0.0011	0.9745	110
4,6-dimethyldecane	0.0010	0.9755	111
ethylcyclopentane	0.0010	0.9765	112
OTHER C9	0.0010	0.9775	113
2,3-dimethylpentane	0.0009	0.9784	114

1,3-dimethyl-4-ethylbenzene	0.0009	0.9793	115
1,1,2-trimethylcyclopentane	0.0009	0.9802	116
3-methylundecane	0.0008	0.9810	117
trans-1-ethyl-2-methylcyclohexane	0.0008	0.9818	118
2,2,3,3-tetramethylhexane	0.0008	0.9826	119
1,3-dimethyl-2-ethylbenzene	0.0007	0.9833	120
(2-methylbutyl)benzene	0.0007	0.9841	121
1,1-dimethylcyclopentane	0.0007	0.9848	122
4-methylheptane	0.0007	0.9855	123
2,5-dimethylheptane	0.0007	0.9862	124
2,6-dimethylundecane	0.0006	0.9868	125
4-methylundecane	0.0006	0.9874	126
(2-methylbutyl)cyclohexane	0.0006	0.9880	127
3-methyldecane	0.0006	0.9886	128
2,6-dimethyldecane	0.0006	0.9892	129
2-methylnonane	0.0006	0.9897	130
1,1,2-trimethylcyclohexane	0.0005	0.9903	131
5-isopropylnonane	0.0005	0.9908	132
1-methyl-4-isopropylcyclohexane	0.0005	0.9912	133
2,3-dimethylhexane	0.0004	0.9917	134
1-ethyl-2-isopropylcyclohexane	0.0004	0.9921	135
3-ethylhexane	0.0004	0.9925	136
cis, cis-1,2,4-trimethylcyclohexane	0.0004	0.9930	137
methanol	0.0004	0.9933	138
OTHER C12	0.0004	0.9937	139
1-methyl-3-butylbenzene	0.0004	0.9941	140
3-ethyl-2-methylpentane	0.0004	0.9944	141
3,3,5-trimethylheptane	0.0004	0.9948	142
naphthalene	0.0004	0.9952	143
isopropylbenzene	0.0004	0.9955	144
methylcyclopentane	0.0003	0.9959	145
5,6-dimethylindane	0.0003	0.9962	146
isobutyl alcohol	0.0003	0.9965	147
3-ethyl-2-methylheptane	0.0003	0.9968	148
1,1,4-trimethylcyclohexane	0.0003	0.9971	149
cis-1-ethyl-2-methylcyclopentane	0.0003	0.9974	150
2,4-dimethylheptane	0.0003	0.9977	151
1,2,3,4-tetramethylcyclohexane	0.0003	0.9979	152
3,4-dimethylhexane	0.0002	0.9982	153
1,1-dimethylcyclohexane	0.0002	0.9984	154
2-butyl-1,3-dimethylcyclohexane	0.0002	0.9986	155
2,3,4-trimethylpentane	0.0002	0.9988	156
OTHER C13	0.0002	0.9990	157
5-methyldodecane	0.0002	0.9992	158
cis-1,4-dimethylcyclohexane	0.0001	0.9993	159
2,2,5-trimethylhexane	0.0001	0.9994	160
1-ethyl-1-methylcyclopentane	0.0001	0.9995	161
cis-1-ethyl-3-methylcyclopentane	0.0001	0.9996	162
trans-1,2-dimethylcyclohexane	0.0001	0.9997	163
trans-1-ethyl-3-methylcyclopentane	0.0001	0.9998	164
OTHER C7	0.0001	0.9998	165
2,4-dimethyloctane	0.0001	0.9999	166
OTHER OTHER C8	0.0001	1.0000	167

Group 3s: Solvent-based Industrial Maintenance Coatings			
Compound	Fraction	cum frac.	# of cmpds.
butyl acetate	0.1287	0.1287	1
2-heptanone	0.1107	0.2394	2
1-butanol	0.0695	0.3089	3
methyl amyl ketone	0.0457	0.3546	4
2-butoxy ethanol	0.0331	0.3877	5
1-methoxy-2-propanol	0.0250	0.4127	6
exxate 600*	0.0241	0.4369	7
ethyl-3-ethoxypropionate	0.0238	0.4606	8
decane	0.0232	0.4839	9
diacetone alcohol	0.0216	0.5055	10
1,2,4-trimethylbenzene	0.0208	0.5262	11
texanol	0.0168	0.5430	12
2-pentanone	0.0150	0.5585	13
methanol	0.0151	0.5737	14
EP	0.0146	0.5882	15
toluene	0.0117	0.6000	16
2,2,4-trimethyl-1,3-pentanediol	0.0114	0.6114	17
methyl propyl ketone	0.0111	0.6225	18
undecane	0.0109	0.6334	19
m-xylene	0.0108	0.6441	20
methyl isobutyl ketone	0.0103	0.6545	21
4-methylnonane	0.0078	0.6622	22
butyl alcohol	0.0076	0.6698	23
methyl propylcyclohexane	0.0065	0.6763	24
1-methoxy-2-acetoxypropane	0.0061	0.6823	25
methy isobutyl ketone	0.0059	0.6883	26
o-xylene	0.0055	0.6938	27
1-methyl-2-isopropylcyclohexane	0.0055	0.6993	28
2,6-dimethyloctane	0.0055	0.7048	29
propylcyclohexane	0.0055	0.7103	30
ethylbenzene	0.0055	0.7157	31
isophorone	0.0053	0.7210	32
1,2,3-trimethylbenzene	0.0051	0.7261	33
1-methyl-3-ethylbenzene	0.0050	0.7310	34
ethylene glycol	0.0048	0.7359	35
1,3,5-trimethylbenzene	0.0048	0.7407	36
diethylcyclohexane	0.0047	0.7454	37
1,3-dimethylbenzene	0.0045	0.7499	38
2,6-dimethylnonane	0.0043	0.7542	39
2-methylnonane	0.0043	0.7585	40
1-methyl-3-isopropylcyclohexane	0.0041	0.7626	41
1-ethyl-2-methylbenzene	0.0041	0.7667	42
methyl ethyl ketone	0.0039	0.7707	43
1-ethyl-3-methylbenzene	0.0039	0.7746	44
octane	0.0039	0.7785	45
p-xylene	0.0039	0.7823	46
nonane	0.0038	0.7861	47
1-ethyl-4-methylbenzene	0.0036	0.7897	48
diethyl fumarate	0.0034	0.7931	49
trans-1-ethyl-4-methylcyclohexane	0.0033	0.7964	50
1,2-dimethylbenzene	0.0033	0.7997	51
1,2-dimethylbenzene	0.0033	0.8030	52
1,1,2,3-tetramethylcyclohexane	0.0033	0.8062	53
2,5-dimethylnonane	0.0030	0.8093	54
3-methyldecane	0.0030	0.8123	55
5-methylnonane	0.0030	0.8153	56
OTHER C11	0.0029	0.8182	57
MAK	0.0029	0.8210	58
dodecane	0.0027	0.8238	59
2-propanol	0.0026	0.8264	60
Bz/12Me2/4Et	0.0026	0.8290	61
2-butanone	0.0026	0.8316	62
3-methylnonane	0.0026	0.8342	63
Bz/1235Me4	0.0025	0.8368	64
trans-decalin	0.0025	0.8393	65
1-ethyl-1,3-dimethylcyclohexane	0.0025	0.8418	66
trans, trans-1,2,4-trimethylcyclohexane	0.0025	0.8443	67
5-methyldecane	0.0025	0.8467	68
1-ethyl-2,4-dimethylcyclohexane	0.0023	0.8490	69
trans, cis-1,2,4-trimethylcyclohexane	0.0023	0.8513	70
4-methyldecane	0.0022	0.8535	71
ethyl propylcyclohexane	0.0022	0.8558	72
1-methyl-4-ethylbenzene	0.0022	0.8580	73
Naphthalene	0.0022	0.8602	74
butylcyclohexane	0.0021	0.8623	75
cis-1-ethyl-3-methylcyclohexane	0.0021	0.8643	76
cis-1,3-dimethylcyclohexane	0.0020	0.8663	77
methylcyclohexane	0.0019	0.8683	78
Bz/13Me2	0.0019	0.8701	79
isobutylcyclohexane	0.0018	0.8720	80
Bz/1245Me4	0.0018	0.8738	81
pentylcyclopentane	0.0018	0.8756	82
Bz/1Me/4Pr	0.0018	0.8774	83
1-methyl-2-ethylbenzene	0.0017	0.8791	84
OTHER C10	0.0016	0.8808	85
1,4-dimethylbenzene	0.0016	0.8823	86
1-methyl-3-isopropylbenzene	0.0016	0.8839	87
BuOH	0.0015	0.8854	88
3,6-dimethyloctane	0.0015	0.8869	89
butylcyclohexane	0.0014	0.8883	90
indane	0.0014	0.8897	91
5-ethyl-3-methyloctane	0.0014	0.8911	92
4-ethyloctane	0.0014	0.8925	93
OTHER C9	0.0014	0.8938	94
Bz/1Me/2iPr	0.0014	0.8952	95
2-methyldecane	0.0013	0.8965	96
2-methylheptane	0.0013	0.8979	97
pentylcyclohexane	0.0013	0.8992	98
Bz/14Me2/2Et	0.0013	0.9005	99
acetone	0.0013	0.9018	100
cis, trans-1,2,4-trimethylcyclohexane	0.0013	0.9031	101
3-ethyl-2-methylheptane	0.0013	0.9044	102
isopropylcyclohexane	0.0013	0.9057	103
neopentyl glycol	0.0013	0.9070	104
cis-decalin	0.0013	0.9082	105
Bz/124Me3	0.0013	0.9095	106
1,2-dimethyl-3-ethylcyclohexane	0.0013	0.9108	107
3,7-dimethylnonane	0.0012	0.9120	108
isopropylbenzene	0.0012	0.9132	109
OTHER C12	0.0012	0.9143	110
1,1,3,5-tetramethylcyclohexane	0.0012	0.9155	111
Bz/1Me/3Pr	0.0012	0.9167	112
cis, trans-1,2,3-trimethylcyclohexane	0.0012	0.9178	113
ethylcyclohexane	0.0012	0.9190	114
1,2,3-trimethylcyclohexane	0.0011	0.9201	115

2,4-dimethylnonane	0.0011	0.9212	116
2-methyldecalin	0.0011	0.9223	117
2,5-dimethyloctane	0.0011	0.9234	118
n-propylbenzene	0.0011	0.9244	119
2,4,6-trimethyloctane	0.0011	0.9255	120
1,1,3-trimethylcyclohexane	0.0010	0.9265	121
1-ethyl-4-isopropylbenzene	0.0010	0.9275	122
Bz/14Et2	0.0010	0.9286	123
1-methyl-4-isopropylcyclohexane	0.0010	0.9296	124
3-methylstyrene	0.0010	0.9305	125
2,7-dimethylnonane	0.0010	0.9315	126
3-methylheptane	0.0010	0.9325	127
isobutyl alcohol	0.0010	0.9334	128
Indane/4Me	0.0010	0.9344	129
Indane/5Me	0.0010	0.9353	130
4-methylstyrene	0.0009	0.9363	131
3,5-dimethyloctane	0.0009	0.9372	132
Bz/123Me3	0.0009	0.9381	133
2,3-dimethyloctane	0.0009	0.9390	134
bicyclo[3.3.1]nonane	0.0009	0.9400	135
4-ethylnonane	0.0009	0.9409	136
methyl isopropylcyclohexane	0.0009	0.9418	137
3,3-dimethyloctane	0.0009	0.9426	138
methyl butylcyclohexane	0.0009	0.9435	139
heptane	0.0008	0.9443	140
cis, cis-1,3,5-trimethylcyclohexane	0.0008	0.9452	141
Bz/1Et/4Pr	0.0008	0.9460	142
1,2,3,5-tetramethylbenzene	0.0008	0.9468	143
cis-1-ethyl-4-methylcyclohexane	0.0008	0.9476	144
5-ethyl-2-methyloctane	0.0008	0.9485	145
1,3-dimethyl-2-isopropylcyclopentane	0.0008	0.9493	146
1-methyl-4-propylbenzene	0.0008	0.9501	147
3-ethyloctane	0.0008	0.9508	148
1,4-dimethyl-1-ethylcyclohexane	0.0008	0.9516	149
2,3,5-trimethylheptane	0.0008	0.9524	150
Bz/Et	0.0007	0.9531	151
3,7-dimethyldecane	0.0007	0.9539	152
trans, trans-1,3,5-trimethylcyclohexane	0.0007	0.9546	153
3-methylundecane	0.0007	0.9553	154
bicyclo[3.3.0]octane	0.0007	0.9560	155
5-methylundecane	0.0007	0.9567	156
trans-1,4-dimethylcyclohexane	0.0007	0.9575	157
trans-1,3-dimethylcyclohexane	0.0007	0.9582	158
Bz/14Me2	0.0007	0.9589	159
EEP	0.0007	0.9595	160
3-methyloctane	0.0007	0.9602	161
2,6-dimethylheptane	0.0007	0.9609	162
1methyl-4-isopropylcyclohexane	0.0007	0.9616	163
propylbenzene	0.0007	0.9622	164
4,5-dimethyldecane	0.0007	0.9629	165
trans-1-ethyl-3-methylcyclohexane	0.0006	0.9635	166
acetophenone	0.0006	0.9642	167
1,4-dimethyl-2-ethylbenzene	0.0006	0.9648	168
1,2-dimethyl-4-ethylbenzene	0.0006	0.9654	169
5-isopropylnonane	0.0006	0.9661	170
4-methylheptane	0.0006	0.9667	171
2-methylundecane	0.0006	0.9673	172
3,4-dimethyloctane	0.0006	0.9679	173
3,3,5-trimethylheptane	0.0006	0.9685	174
4-methyloctane	0.0006	0.9691	175
Bz/12Me2/3Et	0.0006	0.9697	176
5-ethyl-2-methylheptane	0.0006	0.9703	177
1-methyl-3-propylbenzene	0.0006	0.9709	178
cis-1-ethyl-2-methylcyclohexane	0.0006	0.9715	179
Bz/1Me/2Pr	0.0005	0.9720	180
Bz/12Me2	0.0005	0.9725	181
2,5-dimethyldecane	0.0005	0.9731	182
5-methylindane	0.0005	0.9736	183
2,4-dimethyldecane	0.0005	0.9741	184
2,4-dimethyloctane	0.0005	0.9746	185
2,6-dimethyldecane	0.0005	0.9750	186
4-methylundecane	0.0005	0.9755	187
2,2,3,3-tetramethylhexane	0.0005	0.9760	188
3-ethyl-2-methyloctane	0.0005	0.9765	189
trans-bicyclo[4.3.0]nonane	0.0005	0.9769	190
cis, cis-1,2,4-trimethylcyclohexane	0.0004	0.9773	191
Bz/13Et2	0.0004	0.9778	192
3,4-dimethylhexane	0.0004	0.9782	193
butylbenzene	0.0004	0.9786	194
cis-bicyclo[4.3.0]nonane	0.0004	0.9791	195
1,3-diethylbenzene	0.0004	0.9795	196
trans-1-ethyl-2-methylcyclohexane	0.0004	0.9799	197
1,3-dimethyl-2-ethylbenzene	0.0004	0.9803	198
pentylcyclohexane	0.0004	0.9807	199
2-phenyl-2-propanol	0.0004	0.9811	200
2-ethyl-1,3-dimethylcyclohexane	0.0004	0.9815	201
3-ethylnonane	0.0004	0.9818	202
ethanol	0.0004	0.9822	203
2-methylundecane	0.0004	0.9826	204
6-methylundecane	0.0003	0.9829	205
3-methyldecane	0.0003	0.9832	206
4-ethyldecane	0.0003	0.9836	207
sec butylbenzene	0.0003	0.9839	208
sec butylcyclohexane	0.0003	0.9843	209
Bz/12Me2/4Pr	0.0003	0.9846	210
2-butoxyethanol	0.0003	0.9849	211
5-methyldecane	0.0003	0.9852	212
2-methyloctane	0.0003	0.9855	213
4-methylindane	0.0003	0.9858	214
ethyl propylcyclohexane	0.0003	0.9861	215
3,3,4-trimethylheptane	0.0003	0.9864	216
2,4,5-trimethylheptane	0.0003	0.9867	217
Bz/13Me2/5iPr	0.0003	0.9870	218
1,2,4-trimethylcyclopentane	0.0003	0.9873	219
4-methyldecane	0.0003	0.9876	220
4,5-dimethyloctane	0.0003	0.9879	221
Bz/1234Me4	0.0003	0.9882	222
3-ethyldecane	0.0003	0.9884	223
Bz/4Et/123Me3	0.0003	0.9887	224
1-ethyl-2,2,6-trimethylcyclohexane	0.0003	0.9890	225
2,3-dimethyldecane	0.0003	0.9892	226
1,2,3-trimethylcyclopentane	0.0003	0.9895	227
Bz/14iPr2	0.0003	0.9898	228
2,6-dimethylundecane	0.0003	0.9900	229
2,5-dimethylheptane	0.0002	0.9903	230
3,7-dimethylnonane	0.0002	0.9905	231
2,4-dimethylhexane	0.0002	0.9907	232
1,2,4,5-tetramethylbenzene	0.0002	0.9910	233
1-ethyl-1,2-	0.0002	0.9912	234

dimethylcyclohexane			
Bz/1Et/3iPr	0.0002	0.9914	235
6-ethyl-2-methylnonane	0.0002	0.9917	236
2,6-dimethyldecane	0.0002	0.9919	237
Bz/1Me/3Bu	0.0002	0.9921	238
Bz/13Me2/4iPr	0.0002	0.9923	239
cis-1-ethyl-2-methylcyclopentane	0.0002	0.9925	240
OTHER C13	0.0002	0.9927	241
cis-1,4-dimethylcyclohexane	0.0002	0.9928	242
6-methylundecane	0.0002	0.9930	243
1,1-dimethylcyclohexane	0.0002	0.9932	244
Bz/Me5	0.0002	0.9934	245
EtOAc	0.0002	0.9936	246
1-methylindane	0.0002	0.9937	247
2,4-dimethylheptane	0.0002	0.9939	248
C5/2Ph	0.0002	0.9941	249
4,5-dimethylnonane	0.0002	0.9942	250
Bz/135Me3	0.0002	0.9944	251
BuOAc	0.0002	0.9946	252
2,3-dimethylhexane	0.0002	0.9947	253
3-ethylhexane	0.0001	0.9949	254
1,1,3-trimethylcyclopentane	0.0001	0.9950	255
2-methyldecalin	0.0001	0.9951	256
Bz/1Et/3Me	0.0001	0.9953	257
Bz/13Me2/2Et	0.0001	0.9954	258
tert-butyl alcohol	0.0001	0.9956	259
EtOH	0.0001	0.9957	260
1,1,4-trimethylcyclohexane	0.0001	0.9959	261
3,5-dimethyldecane	0.0001	0.9960	262
(2-methylbutyl)cyclohexane	0.0001	0.9961	263
1,2,3,4-tetramethylcyclohexane	0.0001	0.9963	264
1,2,4,5-teramethylbenzene	0.0001	0.9964	265
propylcyclopentane	0.0001	0.9965	266
Bz/1Et/2Me	0.0001	0.9966	267
cis-1,2-dimethylcyclohexane	0.0001	0.9967	268
2,2-dimethylheptane	0.0001	0.9969	269
3,8-dimethyldecane	0.0001	0.9970	270
1,2,3-trimethyl-4-ethylbenzene	0.0001	0.9971	271
2,3-dimethylheptane	0.0001	0.9972	272
tridecane	0.0001	0.9973	273
Bz/1Et/2Pr	0.0001	0.9974	274
cis-1-ethyl-3-methylcyclopentane	0.0001	0.9975	275
1-ethyl-2-isopropylcyclohexane	0.0001	0.9976	276
trans-1-ethyl-3-methylcyclopentane	0.0001	0.9977	277
2-methylhexane	0.0001	0.9978	278
Indane/1Me	0.0001	0.9979	279
2-phenylpentane	0.0001	0.9980	280
trans-1,3-dimethylcyclopentane	0.0001	0.9981	281
Bz/12Et2	0.0001	0.9982	282
Bz/1Et/4iPr	0.0001	0.9983	283
2,5-dimethylhexane	0.0001	0.9983	284
trans-1,2-dimethylcyclohexane	0.0001	0.9984	285
5,6-dimethylindane	0.0001	0.9985	286
C5/3Ph	0.0001	0.9986	287
1,1,5-trimethylindane	0.0001	0.9987	288
cis-1,3-dimethylcyclopentane	0.0001	0.9987	289
4-methylundecane	0.0001	0.9988	290
Bz/1Et/4Me	0.0001	0.9989	291
1,1,2-trimethylcyclopentane	0.0001	0.9990	292
methyl isoamyl ketone	0.0001	0.9990	293
Bz/Me	0.0001	0.9991	294
Indane/47Me2	0.0001	0.9991	295
1-ethyl-4-propylbenzene	0.0001	0.9992	296
Bz/1Me/3iPr	0.0001	0.9993	297
1,1-dimethylcyclopentane	0.0001	0.9993	298
1-ethyl-3-isopropylbenzene	0.0001	0.9994	299
2-methylpentane	0.0001	0.9994	300
1-methyl-2-propylbenzene	0.0001	0.9995	301
methyl pentylcyclohexane	0.0000	0.9995	302
3,3-dimethylhexane	0.0000	0.9996	303
2,6-dimethylundecane	0.0000	0.9996	304
5-sec butylnonane	0.0000	0.9997	305
1,2-dimethylcyclopentane	0.0000	0.9997	306
i-butylbenzene	0.0000	0.9997	307
2,5-dimethylundecane	0.0000	0.9998	308
OTHER C7	0.0000	0.9998	309
3-ethyl-2-methylpentane	0.0000	0.9998	310
1-ethyl-2-propylbenzene	0.0000	0.9999	311
pentylbenzene	0.0000	0.9999	312
s-butylbenzene	0.0000	0.9999	313
1-ethyl-2-isopropylbenzene	0.0000	1.0000	314
1,2-dimethyl-3-ethylbenzene	0.0000	1.0000	315
2-phenyl-2-methylbutane	0.0000	1.0000	316

Group 4s: Solvent-based Medium Gloss/High Gloss			
Compound	Fraction	cum frac.	# of cmpds.
decane	0.0853	0.0853	1
undecane	0.0707	0.1560	2
1,2,4-trimethylbenzene	0.0333	0.1894	3
methyl propylcyclohexane	0.0319	0.2213	4
2,6-dimethylnonane	0.0256	0.2468	5
nonane	0.0228	0.2696	6
2-methylnonane	0.0192	0.2888	7
m-xylene	0.0181	0.3069	8
dodecane	0.0175	0.3244	9
4-methylnonane	0.0174	0.3418	10
propylcyclohexane	0.0172	0.3589	11
2,6-dimethyloctane	0.0170	0.3760	12
ethyl propylcyclohexane	0.0167	0.3927	13
3-methyldecane	0.0162	0.4089	14
1-propoxy-2-propanol	0.0155	0.4244	15
5-methyldecane	0.0154	0.4398	16
1-ethyl-4-methylbenzene	0.0143	0.4541	17
pentylcyclopentane	0.0141	0.4681	18
2-methyldecane	0.0137	0.4818	19
1,2,3-trimethylbenzene	0.0126	0.4945	20
1,3,5-trimethylbenzene	0.0126	0.5071	21
1-methyl-3-isopropylcyclohexane	0.0124	0.5195	22
4-methyldecane	0.0114	0.5309	23
1-ethyl-3-methylbenzene	0.0114	0.5423	24
o-xylene	0.0114	0.5537	25
2-methyldecalin	0.0106	0.5643	26
1-ethyl-2-methylbenzene	0.0104	0.5747	27
isopropylcyclohexane	0.0096	0.5843	28
1-methyl-2-isopropylcyclohexane	0.0093	0.5936	29
3,7-dimethylnonane	0.0093	0.6029	30
2,5-dimethylnonane	0.0091	0.6120	31
3-methylnonane	0.0089	0.6209	32
2,3-dimethyloctane	0.0085	0.6294	33
1,3-dimethyl-5-ethylbenzene	0.0085	0.6379	34
methyl butylcyclohexane	0.0080	0.6459	35
1,1,2,3-tetramethylcyclohexane	0.0076	0.6535	36
trans-decalin	0.0074	0.6608	37
ethylbenzene	0.0071	0.6680	38
1,2-dimethyl-3-ethylcyclohexane	0.0070	0.6750	39
diethylcyclohexane	0.0069	0.6819	40
pentylcyclohexane	0.0069	0.6888	41
p-xylene	0.0067	0.6955	42
isobutylcyclohexane	0.0066	0.7021	43
OTHER C10	0.0065	0.7086	44
OTHER C11	0.0064	0.7151	45
butylcyclohexane	0.0064	0.7215	46
1-methyl-4-isopropylcyclohexane	0.0063	0.7277	47
trans-1-ethyl-4-methylcyclohexane	0.0060	0.7338	48
2-methylundecane	0.0057	0.7395	49
methyl isopropylcyclohexane	0.0055	0.7450	50
3-ethyl-2-methylheptane	0.0051	0.7502	51
1-methyl-3-isopropylbenzene	0.0051	0.7553	52
4,5-dimethyldecane	0.0051	0.7604	53
1,4-dimethyl-2-ethylbenzene	0.0051	0.7655	54
2,6-dimethyldecane	0.0048	0.7703	55
5-methylundecane	0.0048	0.7750	56
3-methylundecane	0.0047	0.7797	57
OTHER C12	0.0046	0.7843	58
2-ethyl-1,3-dimethylcyclohexane	0.0046	0.7889	59
3,6-dimethyloctane	0.0045	0.7934	60
3-ethyloctane	0.0044	0.7978	61
cis-1-ethyl-3-methylcyclohexane	0.0043	0.8021	62
1,2,3,5-tetramethylbenzene	0.0043	0.8064	63
cis-decalin	0.0042	0.8106	64
1,3-dimethyl-2-ethylbenzene	0.0041	0.8147	65
1-methyl-3-propylbenzene	0.0041	0.8188	66
4-methylundecane	0.0041	0.8229	67
3,6-dimethyldecane	0.0041	0.8269	68
1-ethyl-2,4-dimethylcyclohexane	0.0038	0.8308	69
4,6-dimethyldecane	0.0038	0.8346	70
5-isopropylnonane	0.0038	0.8384	71
1-methyl-2-ethylbenzene	0.0037	0.8421	72
3,5-dimethylnonane	0.0037	0.8457	73
2,5-dimethyloctane	0.0036	0.8494	74
4-ethylnonane	0.0036	0.8529	75
1,2-dimethyl-4-ethylbenzene	0.0035	0.8564	76
trans, trans-1,2,4-trimethylcyclohexane	0.0033	0.8597	77
3-methyloctane	0.0033	0.8630	78
4-methyloctane	0.0032	0.8662	79
1-ethyl-4-isopropylbenzene	0.0032	0.8694	80
naphthalene	0.0031	0.8724	81
6-methylundecane	0.0031	0.8755	82
2,4-dimethyloctane	0.0030	0.8784	83
1,2,3-trimethylcyclohexane	0.0029	0.8814	84
methyl pentylcyclohexane	0.0028	0.8842	85
cis-1-ethyl-2-methylcyclohexane	0.0027	0.8869	86
cis, trans-1,2,3-trimethylcyclohexane	0.0026	0.8895	87
cis-1-ethyl-4-methylcyclohexane	0.0026	0.8921	88
1,3-diethylbenzene	0.0025	0.8946	89
propylbenzene	0.0025	0.8971	90
isopentylcyclohexane	0.0025	0.8996	91
4-ethyloctane	0.0024	0.9021	92
octane	0.0024	0.9045	93
3,3,5-trimethylheptane	0.0024	0.9068	94
1,1,3-trimethylcyclohexane	0.0024	0.9092	95
1,2,4,5-tetramethylbenzene	0.0023	0.9116	96
hexylcyclopentane	0.0023	0.9139	97
isopropylbenzene	0.0022	0.9161	98
3,4-dimethyloctane	0.0022	0.9183	99
3,5-dimethyloctane	0.0021	0.9205	100
butylcyclohexane	0.0021	0.9226	101
5-methylindane	0.0021	0.9247	102
1,1-dimethyl-2-propylcyclohexane	0.0020	0.9267	103
trans-1-ethyl-2-methylcyclohexane	0.0020	0.9287	104
4-methylindane	0.0020	0.9306	105
cis, trans-1,2,4-trimethylcyclohexane	0.0019	0.9326	106
indane	0.0019	0.9345	107
3,4-dimethylhexane	0.0019	0.9363	108
trans-1-ethyl-3-methylcyclohexane	0.0018	0.9382	109
1,3-dimethyl-4-ethylbenzene	0.0018	0.9400	110

cis, cis-1,2,4-trimethylcyclohexane	0.0018	0.9417	111
trans, cis-1,2,4-trimethylcyclohexane	0.0017	0.9435	112
3-ethylnonane	0.0017	0.9452	113
2,4-dimethyldecane	0.0017	0.9469	114
1,1,3,4-tetramethylcyclohexane	0.0017	0.9486	115
5-methylnonane	0.0016	0.9503	116
butylbenzene	0.0016	0.9519	117
5-ethyl-2-methylheptane	0.0016	0.9534	118
butylcyclopentane	0.0015	0.9549	119
OTHER C9	0.0015	0.9564	120
(2-methylbutyl)cyclohexane	0.0014	0.9578	121
1-methyl-4-propylbenzene	0.0013	0.9591	122
1-ethyl-1,3-dimethylcyclohexane	0.0013	0.9604	123
2-methyloctane	0.0013	0.9616	124
2,3-dimethylheptane	0.0013	0.9629	125
5-ethyl-2-methyloctane	0.0013	0.9641	126
ethylcyclohexane	0.0012	0.9654	127
1,4-dimethyl-1-ethylcyclohexane	0.0012	0.9666	128
1-methyl-2-isopropylbenzene	0.0012	0.9678	129
2,6-dimethylundecane	0.0011	0.9689	130
6-ethyl-2-methylnonane	0.0011	0.9701	131
2,7-dimethylnonane	0.0011	0.9712	132
1,1,2-trimethylcyclohexane	0.0011	0.9722	133
2,6-dimethylundecane	0.0011	0.9733	134
1-methyl-4-isopropylbenzene	0.0010	0.9743	135
1-methylindane	0.0009	0.9752	136
sec butylcyclopentane	0.0009	0.9761	137
3-ethyl-3-methyloctane	0.0008	0.9769	138
cis-1,2-dimethylcyclohexane	0.0008	0.9778	139
1,2-dimethyl-3-ethylbenzene	0.0008	0.9786	140
2-methylheptane	0.0008	0.9794	141
4-ethyldecane	0.0008	0.9802	142
4,5-dimethyloctane	0.0008	0.9809	143
2,4-dimethylnonane	0.0008	0.9817	144
Indan/5Me	0.0007	0.9824	145
pentylcyclohexane	0.0007	0.9831	146
1-ethyl-1,2-dimethylcyclohexane	0.0007	0.9838	147
toluene	0.0006	0.9844	148
1-ethyl-2-propylbenzene	0.0006	0.9851	149
2,7-dimethyldecane	0.0006	0.9857	150
2,4-dimethylundecane	0.0006	0.9863	151
3,3,4-trimethylheptane	0.0006	0.9868	152
1,1,3,5-tetramethylcyclohexane	0.0006	0.9874	153
3-methylheptane	0.0006	0.9880	154
1,4-diisopropylbenzene	0.0006	0.9885	155
cis, cis-1,3,5-trimethylcyclohexane	0.0006	0.9891	156
trans-bicyclo[4.3.0]nonane	0.0006	0.9897	157
2,3,5-trimethylheptane	0.0006	0.9902	158
3-ethyldecane	0.0005	0.9908	159
2,7-dimethyloctane	0.0005	0.9913	160
trans, trans-1,3,5-trimethylcyclohexane	0.0005	0.9918	161
2-methylundecane	0.0005	0.9924	162
3,5-dimethyldecane	0.0005	0.9929	163
6-ethyl-2-methyloctane	0.0004	0.9933	164
cis-1,3-dimethylcyclohexane	0.0004	0.9937	165
5-sec butylnonane	0.0004	0.9941	166
3-phenylpentane	0.0004	0.9945	167
2,3-dimethylnonane	0.0004	0.9949	168
4-methylundecane	0.0004	0.9953	169

2,4,6-trimethyloctane	0.0003	0.9956	170
4-methylheptane	0.0003	0.9959	171
hexylcyclohexane	0.0003	0.9963	172
3,3-dimethyloctane	0.0003	0.9966	173
1,2,3,4-tetramethylcyclohexane	0.0003	0.9969	174
1,2,3,4-tetramethylbenzene	0.0003	0.9972	175
1-methyl-3-butylbenzene	0.0003	0.9974	176
3-ethyl-4-methylheptane	0.0003	0.9977	177
methylcyclohexane	0.0003	0.9979	178
tridecane	0.0002	0.9982	179
2,3-dimethylhexane	0.0002	0.9984	180
2,4-dimethylpentane	0.0002	0.9986	181
4,5-dimethylnonane	0.0002	0.9988	182
1,3-dimethyl-5-isopropylbenzene	0.0002	0.9989	183
1-ethyl-3-isopropylbenzene	0.0002	0.9991	184
1-ethyl-4-propylbenzene	0.0002	0.9993	185
cyclohexane/1124Me4	0.0002	0.9994	186
OTHER C13	0.0001	0.9996	187
2,5-dimethylheptane	0.0001	0.9997	188
1,1,5-trimethylindane	0.0001	0.9999	189
methyl ethyl ketone	0.0001	1.0000	190

Group 5s: Solvent-based Primers and Sealers			
Compound	Fraction	cum frac.	# of cmpds.
undecane	0.0780	0.0780	1
decane	0.0510	0.1290	2
1,2,4-trimethylbenzene	0.0430	0.1720	3
methyl ethyl ketone	0.0310	0.2031	4
dodecane	0.0246	0.2277	5
2-methyldecalin	0.0195	0.2472	6
toluene	0.0191	0.2663	7
ethyl propylcyclohexane	0.0168	0.2830	8
methylcyclohexane	0.0168	0.2998	9
methyl propylcyclohexane	0.0166	0.3164	10
1-ethyl-3-methylbenzene	0.0160	0.3324	11
2,6-dimethylnonane	0.0151	0.3475	12
1,2,3-trimethylbenzene	0.0148	0.3623	13
1-ethyl-4-methylbenzene	0.0147	0.3770	14
2-methylnonane	0.0146	0.3915	15
1-methyl-2-isopropylcyclohexane	0.0144	0.4059	16
nonane	0.0133	0.4192	17
1,3,5-trimethylbenzene	0.0130	0.4323	18
3-methyldecane	0.0127	0.4449	19
m-xylene	0.0124	0.4574	20
5-methyldecane	0.0124	0.4698	21
propylcyclohexane	0.0124	0.4822	22
methyl butylcyclohexane	0.0120	0.4942	23
4-methylnonane	0.0118	0.5060	24
3,6-dimethyldecane	0.0117	0.5177	25
OTHER C12	0.0114	0.5291	26
2,6-dimethyloctane	0.0112	0.5403	27
1-ethyl-2-methylbenzene	0.0111	0.5514	28
pentylcyclohexane	0.0106	0.5620	29
pentylcyclopentane	0.0099	0.5720	30
2-methylundecane	0.0097	0.5817	31
1-methyl-3-isopropylcyclohexane	0.0095	0.5913	32
diethylcyclohexane	0.0092	0.6005	33
o-xylene	0.0090	0.6095	34
1,4-dimethyl-2-ethylbenzene	0.0084	0.6179	35
3-methylundecane	0.0083	0.6261	36
2,6-dimethyldecane	0.0081	0.6342	37
4-methyldecane	0.0077	0.6419	38
heptane	0.0077	0.6496	39
5-methylindane	0.0075	0.6571	40
isopropylcyclohexane	0.0075	0.6646	41
6-methylundecane	0.0070	0.6716	42
octane	0.0069	0.6786	43
2-methyldecane	0.0068	0.6853	44
trans-decalin	0.0066	0.6920	45
trans-1-ethyl-4-methylcyclohexane	0.0065	0.6985	46
1,2-dimethyl-3-ethylcyclohexane	0.0065	0.7050	47
4-methylundecane	0.0065	0.7114	48
1,3-dimethyl-5-ethylbenzene	0.0065	0.7179	49
OTHER C10	0.0061	0.7240	50
hexylcyclopentane	0.0058	0.7298	51
cis-1-ethyl-3-methylcyclohexane	0.0058	0.7356	52
1,3-dimethyl-2-ethylbenzene	0.0057	0.7413	53
butylcyclohexane	0.0057	0.7470	54
3,7-dimethylnonane	0.0057	0.7527	55
1,2,3-trimethylcyclohexane	0.0054	0.7581	56
1,1,2,3-tetramethylcyclohexane	0.0052	0.7633	57
5-methylundecane	0.0051	0.7684	58
propylbenzene	0.0051	0.7735	59
1,2,4,5-tetramethylbenzene	0.0047	0.7782	60
p-xylene	0.0045	0.7827	61
trans, trans-1,2,4-trimethylcyclohexane	0.0044	0.7871	62
ethylbenzene	0.0044	0.7916	63
4,5-dimethyldecane	0.0043	0.7959	64
naphthalene	0.0040	0.7999	65
2-methylheptane	0.0039	0.8038	66
cis-1,3-dimethylcyclohexane	0.0038	0.8077	67
3-methylnonane	0.0038	0.8115	68
2-propanol	0.0036	0.8151	69
5-ethyl-3-methyloctane	0.0036	0.8187	70
2,5-dimethylnonane	0.0036	0.8223	71
2,3-dimethyloctane	0.0034	0.8257	72
cis-decalin	0.0034	0.8291	73
3,6-dimethyloctane	0.0032	0.8324	74
isobutylcyclohexane	0.0032	0.8355	75
3-methylheptane	0.0032	0.8387	76
methyl pentylcyclohexane	0.0031	0.8418	77
2,4-dimethylnonane	0.0031	0.8450	78
3-ethylnonane	0.0031	0.8480	79
1,2-dimethyl-4-ethylbenzene	0.0031	0.8511	80
2,4-dimethyldecane	0.0030	0.8542	81
OTHER C11	0.0030	0.8572	82
3-ethyl-2-methylheptane	0.0030	0.8601	83
methyl isopropylcyclohexane	0.0030	0.8631	84
2,7-dimethylnonane	0.0029	0.8661	85
2,5-dimethyloctane	0.0026	0.8687	86
4-methyloctane	0.0026	0.8713	87
1-ethyl-4-isopropylbenzene	0.0026	0.8739	88
trans, trans-1,3,5-trimethylcyclohexane	0.0026	0.8765	89
trans-1-ethyl-3-methylcyclohexane	0.0026	0.8791	90
1-cyclopentyl-2-methylpentane	0.0025	0.8816	91
1,1,3-trimethylcyclohexane	0.0025	0.8841	92
6-ethyl-2-methyloctane	0.0024	0.8865	93
5-ethyl-2-methyloctane	0.0024	0.8889	94
3-methyloctane	0.0024	0.8913	95
cis, trans-1,2,3-trimethylcyclohexane	0.0024	0.8937	96
1-methyl-4-isopropylcyclohexane	0.0023	0.8960	97
1-ethyl-2,2,6-trimethylcyclohexane	0.0023	0.8982	98
methylindane	0.0023	0.9005	99
1-ethyl-1,3-dimethylcyclohexane	0.0023	0.9028	100
3-ethyloctane	0.0021	0.9049	101
5,6-dimethylindane	0.0021	0.9070	102
4,5-dimethyloctane	0.0021	0.9090	103
1,1-dimethyl-2-propylcyclohexane	0.0020	0.9110	104
trans, cis-1,2,4-trimethylcyclohexane	0.0020	0.9130	105
isopropylbenzene	0.0019	0.9149	106
ethylcyclohexane	0.0019	0.9168	107
1-methyl-4-propylbenzene	0.0019	0.9187	108
2,7-dimethyldecane	0.0019	0.9205	109
1,3-dimethyl-2-isopropylcyclopentane	0.0018	0.9224	110
2,4-dimethylhexane	0.0017	0.9241	111

OTHER C9	0.0017	0.9258	112
1,3-dimethyl-4-ethylbenzene	0.0017	0.9274	113
4-methylheptane	0.0017	0.9291	114
1,2-diethyl-1-methylcyclohexane	0.0017	0.9307	115
2,7-dimethyloctane	0.0016	0.9324	116
3,8-dimethyldecane	0.0016	0.9340	117
2-ethyl-1,3-dimethylcyclohexane	0.0016	0.9355	118
cis, trans-1,2,4-trimethylcyclohexane	0.0015	0.9371	119
butyl ethylcyclohexane	0.0015	0.9386	120
3,4-dimethylhexane	0.0015	0.9401	121
1,2,4-trimethylcyclopentane	0.0015	0.9416	122
cis-1,2-dimethylcyclohexane	0.0015	0.9430	123
2,3,5-trimethylheptane	0.0014	0.9445	124
cis-1,4-dimethylcyclohexane	0.0014	0.9459	125
2,6-dimethylundecane	0.0014	0.9473	126
1-ethyl-3-isopropylbenzene	0.0014	0.9487	127
indane	0.0014	0.9501	128
trans-1,4-dimethylcyclohexane	0.0014	0.9515	129
4,6-dimethyldecane	0.0014	0.9528	130
1,2,3,4-tetramethylbenzene	0.0013	0.9542	131
6-methyldodecane	0.0013	0.9555	132
1-methyl-4-isopropylbenzene	0.0013	0.9568	133
sec-butylbenzene	0.0013	0.9581	134
1,1,3-trimethylcyclopentane	0.0013	0.9593	135
3,4-dimethyloctane	0.0012	0.9605	136
1-methylindane	0.0012	0.9617	137
1-methyl-3-propylbenzene	0.0012	0.9629	138
1-methyl-3-isopropylbenzene	0.0012	0.9641	139
2,2,3,3-tetramethylpentane	0.0011	0.9652	140
1,2,3-trimethylcyclopentane	0.0011	0.9663	141
2,5-dimethyldecane	0.0011	0.9675	142
1,2-dimethylcyclopentane	0.0011	0.9686	143
butylcyclopentane	0.0011	0.9697	144
2,4-dimethyloctane	0.0010	0.9707	145
5-sec-butylnonane	0.0010	0.9717	146
cis-1-ethyl-4-methylcyclohexane	0.0009	0.9727	147
2,4,6-trimethyloctane	0.0009	0.9736	148
1,1,2-trimethylcyclohexane	0.0009	0.9745	149
trans-1,2-dimethylcyclohexane	0.0009	0.9754	150
3-methylhexane	0.0009	0.9763	151
3,5-dimethyloctane	0.0008	0.9771	152
3,3,5-trimethylheptane	0.0008	0.9779	153
cis-1-ethyl-2-methylcyclohexane	0.0008	0.9787	154
3-ethylhexane	0.0008	0.9795	155
4-ethyloctane	0.0008	0.9803	156
2,5-dimethylhexane	0.0008	0.9811	157
sec butylcyclohexane	0.0008	0.9818	158
5-isopropylnonane	0.0008	0.9826	159
2,6-dimethylundecane	0.0007	0.9833	160
2,5-dimethylheptane	0.0007	0.9840	161
1-methyl-2-propylcyclopentane	0.0007	0.9847	162
4-ethylnonane	0.0007	0.9854	163
3,6-dimethylnonane	0.0006	0.9861	164
cis-1,3-dimethylcyclopentane	0.0006	0.9867	165
2,3-dimethylhexane	0.0006	0.9873	166
3-ethylheptane	0.0006	0.9879	167
2-methyloctane	0.0006	0.9885	168
1,1,2-trimethylcyclopentane	0.0006	0.9890	169
(2-methylbutyl)cyclohexane	0.0005	0.9896	170
hexylcyclohexane	0.0005	0.9901	171
butyl acetate	0.0005	0.9906	172
isobutyl alcohol	0.0005	0.9911	173
butylbenzene	0.0005	0.9916	174
trans-1,3-dimethylcyclopentane	0.0004	0.9921	175
cis, cis-1,2,4-trimethylcyclohexane	0.0004	0.9925	176
1,1-dimethylcyclohexane	0.0004	0.9929	177
2,2,3,3-tetramethylhexane	0.0004	0.9933	178
1-ethyl-1,2-dimethylcyclohexane	0.0004	0.9937	179
2,4-dimethylundecane	0.0004	0.9941	180
2-methylhexane	0.0004	0.9945	181
sec butylbenzene	0.0004	0.9949	182
2,4-dimethylheptane	0.0004	0.9952	183
OTHER C13	0.0003	0.9955	184
cis, cis-1,3,5-trimethylcyclohexane	0.0003	0.9959	185
styrene	0.0003	0.9962	186
4-ethyldecane	0.0003	0.9965	187
acetone	0.0003	0.9967	188
2,3,4-trimethylpentane	0.0003	0.9970	189
2,9-dimethylundecane	0.0003	0.9973	190
2,2,5-trimethylhexane	0.0002	0.9975	191
1,1,4-trimethylcyclohexane	0.0002	0.9977	192
2,3-dimethylheptane	0.0002	0.9980	193
3,3-dimethyloctane	0.0002	0.9981	194
cis-1-ethyl-3-methylcyclopentane	0.0002	0.9983	195
cis-1-ethyl-2-methylcyclopentane	0.0002	0.9985	196
3-ethyl-2-methylpentane	0.0002	0.9987	197
4-methylindane	0.0002	0.9988	198
2,3-dimethylpentane	0.0002	0.9990	199
cis-bicyclo[3.3.0]octane	0.0001	0.9991	200
trans-1-ethyl-2-methylcyclohexane	0.0001	0.9992	201
OTHER C8	0.0001	0.9994	202
trans-1,3-dimethylcyclohexane	0.0001	0.9995	203

Group 6s: Solvent based Semi-transparent Stains			
Compound	Fraction	cum frac.	# of cmpds.
undecane	0.1028	0.1028	1
1,2,4-trimethylbenzene	0.0567	0.1595	2
1-ethyl-3-methylbenzene	0.0537	0.2133	3
1,3,5-trimethylbenzene	0.0338	0.2471	4
dodecane	0.0326	0.2798	5
3,6-dimethyldecane	0.0312	0.3110	6
1-ethyl-4-methylbenzene	0.0269	0.3379	7
ethyl propylcyclohexane	0.0249	0.3628	8
1-ethyl-2-methylbenzene	0.0240	0.3868	9
2-methyldecalin	0.0230	0.4098	10
decane	0.0221	0.4320	11
cis-decalin	0.0213	0.4533	12
pentylcyclohexane	0.0200	0.4733	13
3-methyldecane	0.0186	0.4919	14
propylbenzene	0.0181	0.5100	15
5-methyldecane	0.0152	0.5252	16
1,2,3-trimethylbenzene	0.0139	0.5391	17
3,7-dimethyldecane	0.0122	0.5513	18
OTHER C12	0.0114	0.5626	19
2-methylundecane	0.0108	0.5734	20
3-methylundecane	0.0104	0.5838	21
diethylcyclohexane	0.0102	0.5940	22
OTHER C13	0.0097	0.6038	23
nonane	0.0096	0.6134	24
methyl butylcyclohexane	0.0093	0.6226	25
2-methyl-6-ethyloctane	0.0091	0.6318	26
o-xylene	0.0088	0.6405	27
4-methylundecane	0.0082	0.6488	28
5-methylundecane	0.0082	0.6570	29
1,4-dimethyl-2-ethylbenzene	0.0080	0.6650	30
1,3-dimethyl-5-ethylbenzene	0.0077	0.6726	31
methyl propylcyclohexane	0.0075	0.6802	32
4-methyldecane	0.0075	0.6877	33
6-ethyl-2-methyloctane	0.0072	0.6949	34
2,6-dimethylnonane	0.0071	0.7020	35
isopropylbenzene	0.0071	0.7091	36
5,6-dimethylindane	0.0069	0.7160	37
4-methylindane	0.0068	0.7229	38
m-xylene	0.0068	0.7296	39
6-methylundecane	0.0066	0.7362	40
2,4-dimethyldecane	0.0065	0.7427	41
trans-decalin	0.0064	0.7492	42
naphthalene	0.0064	0.7556	43
hexylcyclopentane	0.0063	0.7619	44
2-methyldecane	0.0062	0.7682	45
2,6-dimethyloctane	0.0060	0.7742	46
pentylcyclopentane	0.0059	0.7801	47
1-methyl-3-isopropylcyclohexane	0.0056	0.7857	48
5-isopropylnonane	0.0055	0.7912	49
propylcyclohexane	0.0053	0.7965	50
3,7-dimethylnonane	0.0052	0.8018	51
5-methylindane	0.0048	0.8066	52
tridecane	0.0047	0.8112	53
1,3-dimethyl-2-ethylbenzene	0.0045	0.8157	54
1,2-dimethyl-4-ethylbenzene	0.0045	0.8202	55
cis, trans-1,2,4-trimethylcyclohexane	0.0043	0.8245	56
butyl methylcyclohexane	0.0041	0.8285	57
methyl pentylcyclohexane	0.0039	0.8325	58
1,1,2,3-tetramethylcyclohexane	0.0039	0.8364	59
2,6-dimethylundecane	0.0039	0.8402	60
4,5-dimethyldecane	0.0038	0.8440	61
2-methylnonane	0.0036	0.8476	62
1,3-dimethyl-4-isopropylbenzene	0.0036	0.8512	63
2,7-dimethyldecane	0.0034	0.8547	64
OTHER C14	0.0033	0.8580	65
1,2,3-trimethylcyclohexane	0.0032	0.8612	66
hexylcyclohexane	0.0032	0.8645	67
isopropylcyclohexane	0.0032	0.8676	68
indane	0.0032	0.8708	69
3,5-dimethyldecane	0.0031	0.8739	70
cis-1-ethyl-3-methylcyclohexane	0.0030	0.8769	71
2,4-dimethyloctane	0.0030	0.8799	72
2-ethyl-1,3-dimethylcyclohexane	0.0029	0.8828	73
1-methyl-3-propylbenzene	0.0029	0.8857	74
ethylbenzene	0.0028	0.8884	75
4-ethylnonane	0.0027	0.8912	76
2,6-dimethyldecane	0.0027	0.8939	77
1,1-dimethyl-2-propylcyclohexane	0.0026	0.8965	78
2,6-dimethylundecane	0.0025	0.8990	79
cis-bicyclo[4.3.0]nonane	0.0025	0.9015	80
OTHER C10	0.0023	0.9038	81
5-ethyldecane	0.0022	0.9060	82
toluene	0.0021	0.9081	83
1-methyl-2-isopropylcyclohexane	0.0021	0.9101	84
p-xylene	0.0020	0.9122	85
1,3-diethylbenzene	0.0020	0.9142	86
3-methyldodecane	0.0020	0.9161	87
trans, trans-1,2,4-trimethylcyclohexane	0.0019	0.9181	88
2,5-dimethylnonane	0.0019	0.9199	89
2,3-dimethylnonane	0.0019	0.9218	90
1,2,3,4-tetramethylbenzene	0.0018	0.9236	91
4-ethyldecane	0.0018	0.9254	92
2,3-dimethyloctane	0.0018	0.9272	93
OTHER C11	0.0017	0.9289	94
2,6-dimethyldodecane	0.0017	0.9306	95
3,6-dimethyloctane	0.0017	0.9323	96
octane	0.0016	0.9340	97
1,1,5-trimethylindane	0.0016	0.9356	98
2-butyl-1,1,3-trimethylcyclohexane	0.0016	0.9372	99
cis-1-ethyl-2-methylcyclohexane	0.0016	0.9387	100
butylcyclohexane	0.0016	0.9403	101
3-methylnonane	0.0016	0.9419	102
4-methylnonane	0.0015	0.9434	103
2,10-dimethylundecane	0.0014	0.9448	104
1,2,3,5-tetramethylbenzene	0.0014	0.9462	105
3,6-dimethylundecane	0.0014	0.9476	106
tetralin	0.0014	0.9489	107
isobutylcyclohexane	0.0013	0.9503	108
6-methyldodecane	0.0013	0.9516	109
2,7,10-trimethylundecane	0.0013	0.9529	110
1,1,3-trimethylcyclohexane	0.0013	0.9542	111
trans, trans-1,3,5-trimethylcyclohexane	0.0012	0.9554	112
4-methyldodecane	0.0012	0.9566	113
ethylcyclohexane	0.0012	0.9578	114
trans-1-ethyl-4-	0.0012	0.9589	115

methylcyclohexane			
2,6-dimethylheptane	0.0012	0.9601	116
1-methyl-3-isopropylbenzene	0.0011	0.9612	117
3-methyloctane	0.0011	0.9623	118
4,5-dimethylundecane	0.0011	0.9634	119
1-methyl-2-propylbenzene	0.0011	0.9645	120
1,3-dimethyl-4-ethylbenzene	0.0011	0.9656	121
4-methyloctane	0.0011	0.9667	122
1,1,3,4-tetramethylcyclohexane	0.0010	0.9677	123
trans-1-ethyl-2-methylcyclohexane	0.0010	0.9687	124
2,4-dimethylundecane	0.0010	0.9697	125
trans-1-ethyl-3-methylcyclohexane	0.0010	0.9707	126
1-methyl-4-isopropylbenzene	0.0009	0.9716	127
4-ethylundecane	0.0009	0.9726	128
cis, cis-1,2,4-trimethylcyclohexane	0.0009	0.9735	129
1-ethyl-1,3-dimethylcyclohexane	0.0009	0.9744	130
trans, cis-1,2,4-trimethylcyclohexane	0.0009	0.9753	131
4,5-dimethylnonane	0.0009	0.9762	132
2,9-dimethylundecane	0.0009	0.9770	133
1-methyl-2-isopropylbenzene	0.0009	0.9779	134
sec-butylbenzene	0.0009	0.9788	135
2-methyloctane	0.0009	0.9796	136
3-ethylundecane	0.0009	0.9805	137
1,3,5-triethylbenzene	0.0008	0.9813	138
2-methylnaphthalene	0.0008	0.9822	139
3,5-dimethyloctane	0.0008	0.9830	140
2,7-dimethylundecane	0.0008	0.9838	141
3-ethyloctane	0.0008	0.9847	142
(4-methylpentyl)cyclohexane	0.0008	0.9855	143
5-methyltridecane	0.0007	0.9862	144
2,3-dimethylheptane	0.0007	0.9869	145
cis, cis-1,3,5-trimethylcyclohexane	0.0007	0.9876	146
2,7-dimethylnonane	0.0007	0.9883	147
pentamethylbenzene	0.0007	0.9890	148
OTHER C9	0.0007	0.9897	149
1,2,4,5-tetramethylbenzene	0.0007	0.9904	150
2-ethyltetralin	0.0006	0.9910	151
5-methyldodecane	0.0006	0.9916	152
2,5-dimethylundecane	0.0006	0.9923	153
cis-1-ethyl-4-methylcyclohexane	0.0006	0.9929	154
cis, trans-1,2,3-trimethylcyclohexane	0.0006	0.9935	155
1,3-dimethyl-2-isopropylcyclopentane	0.0006	0.9940	156
cis-1,3-dimethylcyclohexane	0.0005	0.9946	157
butylcyclopentane	0.0004	0.9950	158
2,5-dimethyloctane	0.0004	0.9954	159
(2-methylbutyl)cyclohexane	0.0004	0.9958	160
3,4-dimethyloctane	0.0004	0.9961	161
4,7-dimethylindane	0.0004	0.9965	162
2,7-dimethyloctane	0.0004	0.9969	163
trans-1,4-dimethylcyclohexane	0.0004	0.9972	164
1,1,4-trimethylcyclohexane	0.0004	0.9976	165
1-methyl-4-isopropylcyclohexane	0.0003	0.9979	166
2,3,5-trimethylheptane	0.0003	0.9982	167
3-ethyl-2-methylheptane	0.0003	0.9985	168
1-methyl-2-propylcyclopentane	0.0003	0.9988	169
2,7-dimethylheptane	0.0003	0.9991	170
cis-1,4-dimethylcyclohexane	0.0003	0.9994	171
2-methyltridecane	0.0002	0.9996	172
methylcyclohexane	0.0002	0.9998	173
2-methylheptane	0.0002	1.0000	174

Group 7s: Solvent-based Traffic Paint			
Compound	Fraction	cum frac.	# of cmpds.
octane	0.0559	0.0559	1
decane	0.0550	0.1109	2
undecane	0.0360	0.1469	3
1,2,4-trimethylbenzene	0.0318	0.1787	4
cis-1,3-dimethylcyclohexane	0.0298	0.2085	5
m-xylene	0.0247	0.2332	6
trans, trans-1,2,4-trimethylcyclohexane	0.0233	0.2565	7
4-methylnonane	0.0232	0.2797	8
5-methylnonane	0.0220	0.3017	9
o-xylene	0.0194	0.3211	10
2-methylheptane	0.0191	0.3401	11
2,6-dimethylnonane	0.0169	0.3570	12
ethylcyclohexane	0.0166	0.3737	13
1-ethyl-4-methylbenzene	0.0157	0.3894	14
1-ethyl-2-methylbenzene	0.0154	0.4048	15
propylcyclohexane	0.0153	0.4201	16
trans, cis-1,2,4-trimethylcyclohexane	0.0147	0.4348	17
3-methylheptane	0.0139	0.4487	18
cis-1,4-dimethylcyclohexane	0.0131	0.4618	19
2,6-dimethyloctane	0.0128	0.4747	20
cis-1,2-dimethylcyclohexane	0.0126	0.4873	21
butylcyclohexane	0.0122	0.4995	22
5-methyldecane	0.0116	0.5111	23
1-ethyl-3-methylbenzene	0.0114	0.5225	24
1,2-dimethyl-3-ethylcyclohexane	0.0113	0.5338	25
trans-1,4-dimethylcyclohexane	0.0111	0.5449	26
p-xylene	0.0109	0.5558	27
1,1,3-trimethylcyclohexane	0.0107	0.5665	28
trans-1-ethyl-4-methylcyclohexane	0.0107	0.5772	29
cis-1-ethyl-3-methylcyclohexane	0.0105	0.5877	30
dodecane	0.0105	0.5982	31
1,2-dimethyl-3-ethylcyclohexane	0.0104	0.6086	32
ethylbenzene	0.0103	0.6189	33
nonane	0.0102	0.6291	34
trans, trans-1,3,5-trimethylcyclohexane	0.0099	0.6390	35
3-methyldecane	0.0096	0.6486	36
3-ethylnonane	0.0094	0.6581	37
1-methyl-3-isopropylcyclohexane	0.0087	0.6668	38
3,6-dimethylnonane	0.0084	0.6751	39
cis-decalin	0.0081	0.6833	40
sec butylcyclohexane	0.0078	0.6911	41
isopropylcyclohexane	0.0078	0.6989	42
cis, trans-1,2,4-trimethylcyclohexane	0.0077	0.7066	43
trans-decalin	0.0077	0.7143	44
2,5-dimethylnonane	0.0075	0.7218	45
1,2-dimethyl-3-ethylcyclohexane	0.0072	0.7290	46
1,2,3-trimethylbenzene	0.0069	0.7359	47
3-methyloctane	0.0067	0.7426	48
5-ethyl-3-methyloctane	0.0067	0.7493	49
4-methyldecane	0.0066	0.7560	50
2,5-dimethylheptane	0.0063	0.7623	51
2-methyldecalin	0.0063	0.7685	52
2-methyloctane	0.0062	0.7748	53
4,5-dimethylnonane	0.0061	0.7808	54
3,7-dimethylnonane	0.0059	0.7867	55
4-methylheptane	0.0059	0.7926	56
2-methylnonane	0.0058	0.7985	57
1-methyl-3-isopropylcyclohexane	0.0058	0.8043	58
4-ethylnonane	0.0057	0.8100	59
2,5-dimethyldecane	0.0057	0.8156	60
2-methyldecalin	0.0056	0.8213	61
isobutylcyclohexane	0.0055	0.8268	62
3-ethyl-2-methylheptane	0.0054	0.8322	63
diethylcyclohexane	0.0053	0.8375	64
1-methyl-4-isopropylcyclohexane	0.0051	0.8427	65
methyl propylcyclohexane	0.0051	0.8478	66
OTHER C9	0.0051	0.8529	67
methyl propylcyclohexane	0.0050	0.8579	68
4-methyloctane	0.0045	0.8624	69
1,2-diethyl-1-methylcyclohexane	0.0044	0.8668	70
pentylcyclohexane	0.0042	0.8710	71
3,3,5-trimethylheptane	0.0041	0.8751	72
methyl propylcyclohexane	0.0041	0.8792	73
hexylcyclopentane	0.0039	0.8831	74
2,5-dimethyloctane	0.0039	0.8870	75
3,6-dimethyloctane	0.0039	0.8909	76
cis, trans-1,2,3-trimethylcyclohexane	0.0038	0.8948	77
1-ethyl-2,2,6-trimethylcyclohexane	0.0036	0.8984	78
trans-bicyclo[4.3.0]nonane	0.0036	0.9020	79
OTHER C10	0.0035	0.9055	80
2,3,5-trimethylheptane	0.0035	0.9090	81
3-methylundecane	0.0033	0.9123	82
2-methylundecane	0.0033	0.9157	83
2,4-dimethylheptane	0.0032	0.9189	84
1,1-dimethylcyclohexane	0.0032	0.9221	85
2-ethyl-1,3-dimethylcyclohexane	0.0030	0.9250	86
1-methyl-2-isopropylcyclohexane	0.0029	0.9279	87
1,3,5-trimethylbenzene	0.0028	0.9307	88
6-methylundecane	0.0027	0.9334	89
3-ethylhexane	0.0027	0.9361	90
cis-1-ethyl-2-methylcyclopentane	0.0027	0.9387	91
4-methylundecane	0.0026	0.9413	92
1,1,4-trimethylcyclohexane	0.0024	0.9437	93
ethyl propylcyclohexane	0.0023	0.9460	94
cis-1-ethyl-4-methylcyclohexane	0.0023	0.9483	95
ethyl propylcyclohexane	0.0023	0.9506	96
propylbenzene	0.0023	0.9528	97
1,1-dimethyl-2-propylcyclohexane	0.0022	0.9550	98
1,2,4-trimethylcyclopentane	0.0021	0.9571	99
2,3-dimethylhexane	0.0021	0.9592	100
diethylcyclohexane	0.0021	0.9613	101
methylcyclohexane	0.0021	0.9634	102
3,3-dimethyloctane	0.0021	0.9655	103
3-ethyloctane	0.0020	0.9675	104
1,2,3-trimethylcyclopentane	0.0020	0.9695	105
2,2,5-trimethylhexane	0.0019	0.9714	106
ethyl propylcyclohexane	0.0019	0.9733	107

diethylcyclohexane	0.0019	0.9752	108
cis-bicyclo[3.3.0]octane	0.0018	0.9769	109
methyl butylcyclohexane	0.0017	0.9786	110
5-methylundecane	0.0016	0.9802	111
cis-1-ethyl-3-methylcyclopentane	0.0014	0.9817	112
cis, cis-1,2,4-trimethylcyclohexane	0.0014	0.9831	113
OTHER C8	0.0014	0.9845	114
trans-1-ethyl-3-methylcyclopentane	0.0014	0.9859	115
OTHER C9	0.0014	0.9873	116
3,4-dimethylhexane	0.0013	0.9886	117
2,6-dimethylundecane	0.0013	0.9899	118
1,1,2-trimethylcyclopentane	0.0013	0.9912	119
toluene	0.0013	0.9925	120
1,2,3-trimethylcyclohexane	0.0013	0.9938	121
OTHER C9	0.0012	0.9950	122
2,4-dimethylhexane	0.0011	0.9961	123
trans-1,2-dimethylcyclohexane	0.0011	0.9972	124
1-ethyl-1-methylcyclopentane	0.0011	0.9983	125
3,5-dimethyloctane	0.0009	0.9992	126
trans-1-ethyl-3-methylcyclohexane	0.0008	1.0000	127

Group 8s: Solvent-based Varnishes			
Compound	Fraction	cum frac.	# of cmpds.
decane	0.0949	0.0949	1
1,2,4-trimethylbenzene	0.0483	0.1432	2
undecane	0.0391	0.1823	3
2-methylnonane	0.0340	0.2164	4
2,6-dimethylnonane	0.0284	0.2447	5
methyl propylcyclohexane	0.0259	0.2707	6
nonane	0.0252	0.2959	7
diethylcyclohexane	0.0230	0.3190	8
dodecane	0.0223	0.3412	9
2,6-dimethyloctane	0.0219	0.3631	10
1-ethyl-4-methylbenzene	0.0211	0.3842	11
1,3,5-trimethylbenzene	0.0195	0.4037	12
propylcyclohexane	0.0194	0.4230	13
1,1,2,3-tetramethylcyclohexane	0.0177	0.4407	14
1-ethyl-3-methylbenzene	0.0174	0.4582	15
1-methyl-3-isopropylcyclohexane	0.0166	0.4748	16
3-methylnonane	0.0164	0.4911	17
4-methylnonane	0.0161	0.5072	18
5-methyldecane	0.0156	0.5228	19
1-ethyl-2-methylbenzene	0.0146	0.5374	20
3,7-dimethylnonane	0.0136	0.5510	21
pentylcyclopentane	0.0129	0.5639	22
1,2,3-trimethylbenzene	0.0125	0.5764	23
2-methyldecane	0.0118	0.5882	24
4-methyldecane	0.0111	0.5993	25
1,3-dimethyl-5-ethylbenzene	0.0108	0.6101	26
2,4-dimethyloctane	0.0107	0.6208	27
1-methyl-2-isopropylbenzene	0.0102	0.6310	28
1,3-dimethyl-2-isopropylcyclopentane	0.0098	0.6408	29
3-methyldecane	0.0097	0.6505	30
isopropylcyclohexane	0.0095	0.6601	31
ethyl propylcyclohexane	0.0093	0.6693	32
propylbenzene	0.0089	0.6782	33
m-xylene	0.0085	0.6866	34
methyl butylcyclohexane	0.0083	0.6949	35
1-methyl-2-isopropylcyclohexane	0.0083	0.7032	36
1,2,3-trimethylcyclohexane	0.0079	0.7111	37
2-methyldecalin	0.0078	0.7189	38
5-methylindane	0.0077	0.7266	39
o-xylene	0.0076	0.7342	40
cis-bicyclo[4.3.0]nonane	0.0076	0.7418	41
2-ethyl-1,3-dimethylcyclohexane	0.0071	0.7490	42
1,4-dimethyl-2-ethylbenzene	0.0070	0.7560	43
cis-1-ethyl-3-methylcyclohexane	0.0070	0.7630	44
4-ethylnonane	0.0069	0.7698	45
5-isopropylnonane	0.0062	0.7760	46
OTHER C11	0.0052	0.7812	47
1,3-dimethyl-2-ethylbenzene	0.0051	0.7864	48
3,6-dimethyloctane	0.0051	0.7914	49
1-ethyl-4-isopropylbenzene	0.0050	0.7964	50
1,2,3,4-tetramethylbenzene	0.0049	0.8014	51
isobutylcyclohexane	0.0046	0.8060	52
cis, cis-1,2,4-trimethylcyclohexane	0.0046	0.8106	53
3,5-dimethyloctane	0.0044	0.8150	54
cis-1-ethyl-2-methylcyclohexane	0.0044	0.8195	55
pentylcyclohexane	0.0043	0.8238	56
ethylbenzene	0.0043	0.8280	57
2,6-dimethyldecane	0.0042	0.8322	58
1,3-diethylbenzene	0.0041	0.8364	59
cis-decalin	0.0041	0.8405	60
trans, trans-1,3,5-trimethylcyclohexane	0.0041	0.8445	61
ethanol	0.0041	0.8486	62
1-methyl-4-isopropylbenzene	0.0040	0.8526	63
1-ethyl-1,3-dimethylcyclohexane	0.0037	0.8564	64
3,4-dimethyloctane	0.0037	0.8601	65
2-methylundecane	0.0037	0.8637	66
3,7-dimethyldecane	0.0036	0.8674	67
4-methyloctane	0.0035	0.8709	68
3-methyloctane	0.0034	0.8743	69
butylcyclohexane	0.0034	0.8777	70
2,5-dimethyldecane	0.0033	0.8810	71
1-methyl-3-isopropylbenzene	0.0033	0.8843	72
3-methylundecane	0.0033	0.8876	73
4,5-dimethylnonane	0.0032	0.8908	74
isopropylbenzene	0.0032	0.8940	75
p-xylene	0.0032	0.8972	76
1-methyl-4-isopropylcyclohexane	0.0031	0.9003	77
1,2-dimethyl-4-ethylbenzene	0.0031	0.9034	78
OTHER C10	0.0029	0.9063	79
2,5-dimethylnonane	0.0029	0.9093	80
trans-1-ethyl-2-methylcyclohexane	0.0029	0.9121	81
3,5-dimethyldecane	0.0029	0.9150	82
2,4,6-trimethyloctane	0.0028	0.9178	83
OTHER C9	0.0028	0.9206	84
cis-1-ethyl-4-methylcyclohexane	0.0028	0.9234	85
2,5-dimethyloctane	0.0028	0.9262	86
3-ethyloctane	0.0028	0.9289	87
OTHER C12	0.0027	0.9316	88
1,2,4,5-tetramethylbenzene	0.0026	0.9342	89
1-ethyl-1-methylcyclohexane	0.0025	0.9367	90
1,1,2,3-teramethylcyclohexane	0.0025	0.9392	91
trans-decalin	0.0024	0.9416	92
1,2,3,5-tetramethylbenzene	0.0023	0.9439	93
1,1,3-trimethylcyclohexane	0.0023	0.9462	94
octane	0.0023	0.9485	95
1,1-dimethyl-2-propylcyclohexane	0.0022	0.9507	96
(2-methylbutyl)cyclohexane	0.0021	0.9527	97
hexylcyclopentane	0.0020	0.9547	98
3,3,5-trimethylheptane	0.0020	0.9567	99
tetralin	0.0018	0.9585	100
2,3-dimethylheptane	0.0017	0.9602	101
3,6-dimethyldecane	0.0017	0.9619	102
4,6-dimethyldecane	0.0015	0.9634	103
6-methylundecane	0.0015	0.9649	104
4-ethyldecane	0.0013	0.9662	105
trans-1,2-dimethylcyclohexane	0.0013	0.9675	106
3,6-dimethylnonane	0.0012	0.9687	107
1-methylindane	0.0012	0.9700	108
ethylcyclohexane	0.0012	0.9712	109
2-methyloctane	0.0012	0.9724	110
2,6-dimethylundecane	0.0011	0.9735	111
2,7-dimethyldecane	0.0011	0.9746	112
5-methylundecane	0.0011	0.9757	113
3-ethyl-2-methylheptane	0.0011	0.9767	114

2,6-dimethylheptane	0.0011	0.9778	115
4,5-dimethyloctane	0.0010	0.9788	116
3-ethylnonane	0.0010	0.9798	117
naphthalene	0.0010	0.9808	118
4-methylindane	0.0009	0.9818	119
sec-butylbenzene	0.0009	0.9827	120
4-ethyloctane	0.0009	0.9835	121
cis, trans-1,2,4-trimethylcyclohexane	0.0008	0.9844	122
4-methylundecane	0.0008	0.9852	123
1,1,3,4-tetramethylcyclohexane	0.0007	0.9859	124
1,1,2-trimethylcyclohexane	0.0007	0.9867	125
2,4-dimethylnonane	0.0007	0.9874	126
cis, trans-1,2,3-trimethylcyclohexane	0.0007	0.9881	127
(2-methylbutyl)benzene	0.0007	0.9888	128
2,4-dimethyldecane	0.0007	0.9894	129
toluene	0.0006	0.9900	130
acetone	0.0006	0.9906	131
methyl ethyl ketone	0.0006	0.9912	132
methyl pentylcyclohexane	0.0006	0.9918	133
1,3-dimethyl-4-ethylbenzene	0.0006	0.9924	134
trans-1-ethyl-4-methylcyclohexane	0.0005	0.9929	135
trans-1-ethyl-3-methylcyclohexane	0.0005	0.9934	136
1,1,2-trimethylcyclopentane	0.0005	0.9939	137
3,3-dimethyloctane	0.0005	0.9943	138
1-methyl-2-ethylbenzene	0.0004	0.9948	139
2,5-dimethylundecane	0.0004	0.9952	140
2-methylheptane	0.0004	0.9956	141
3,4-dimethylhexane	0.0004	0.9959	142
2-propanol	0.0004	0.9963	143
4,5-dimethyldecane	0.0003	0.9966	144
2,4-dimethylundecane	0.0003	0.9969	145
trans, trans-1,2,4-trimethylcyclohexane	0.0003	0.9972	146
2,5-dimethylheptane	0.0003	0.9975	147
2,3,5-trimethylheptane	0.0003	0.9977	148
trans, cis-1,2,4-trimethylcyclohexane	0.0003	0.9980	149
OTHER C8	0.0002	0.9982	150
trans-1,4-dimethylcyclohexane	0.0002	0.9984	151
cis, cis-1,3,5-trimethylcyclohexane	0.0002	0.9986	152
OTHER C7	0.0002	0.9987	153
cis-1,3-dimethylcyclohexane	0.0002	0.9989	154
methylcyclohexane	0.0002	0.9991	155

Group 9s: Solvent-based Quick-dry Primers and Non-flats			
Compound	Fraction	cum frac.	# of cmpds.
decane	0.0861	0.0861	1
undecane	0.0439	0.1299	2
methyl propylcyclohexane	0.0380	0.1679	3
1,2,4-trimethylbenzene	0.0340	0.2019	4
octane	0.0249	0.2268	5
2-methylnonane	0.0231	0.2499	6
propylcyclohexane	0.0209	0.2708	7
m-xylene	0.0192	0.2899	8
2,6-dimethyloctane	0.0187	0.3087	9
1-methyl-2-isopropylcyclohexane	0.0174	0.3261	10
1-methyl-3-isopropylcyclohexane	0.0172	0.3433	11
1,1,2,3-tetramethylcyclohexane	0.0162	0.3594	12
nonane	0.0161	0.3755	13
diethylcyclohexane	0.0158	0.3913	14
ethyl propylcyclohexane	0.0142	0.4055	15
4-methylnonane	0.0141	0.4196	16
2,6-dimethylnonane	0.0137	0.4333	17
pentylcyclopentane	0.0130	0.4463	18
1,3,5-trimethylbenzene	0.0125	0.4588	19
o-xylene	0.0122	0.4710	20
cis-1,3-dimethylcyclohexane	0.0122	0.4832	21
1-ethyl-4-methylbenzene	0.0121	0.4953	22
trans, trans-1,2,4-trimethylcyclohexane	0.0117	0.5069	23
2-methylheptane	0.0110	0.5179	24
2,4,6-trimethyloctane	0.0109	0.5288	25
3-methyldecane	0.0109	0.5397	26
trans-decalin	0.0107	0.5504	27
dodecane	0.0102	0.5606	28
3-methylnonane	0.0100	0.5706	29
trans-1-ethyl-4-methylcyclohexane	0.0100	0.5806	30
2,5-dimethylnonane	0.0098	0.5904	31
OTHER C10	0.0098	0.6002	32
1,2-dimethyl-3-ethylcyclohexane	0.0097	0.6099	33
3-methylheptane	0.0093	0.6192	34
2-methyldecane	0.0093	0.6285	35
isopropylcyclohexane	0.0083	0.6367	36
5-methylnonane	0.0079	0.6446	37
5-methyldecane	0.0078	0.6524	38
p-xylene	0.0076	0.6600	39
4-methyldecane	0.0075	0.6675	40
ethylbenzene	0.0074	0.6749	41
3,7-dimethylnonane	0.0073	0.6822	42
1,2,3-trimethylbenzene	0.0072	0.6895	43
1-ethyl-2-methylbenzene	0.0071	0.6966	44
1-ethyl-3-methylbenzene	0.0070	0.7036	45
ethylcyclohexane	0.0066	0.7102	46
2-methyldecalin	0.0065	0.7167	47
butylcyclohexane	0.0065	0.7232	48
cis-1-ethyl-3-methylcyclohexane	0.0063	0.7295	49
4-ethylnonane	0.0061	0.7356	50
1,2,3-trimethylcyclohexane	0.0060	0.7416	51
isobutylcyclohexane	0.0057	0.7473	52
2,7-dimethylnonane	0.0057	0.7530	53
3,6-dimethyloctane	0.0055	0.7586	54
1-methyl-2-ethylbenzene	0.0052	0.7638	55
trans-1,3-dimethylcyclohexane	0.0052	0.7689	56
1,1,3-trimethylcyclohexane	0.0051	0.7741	57
pentylcyclohexane	0.0051	0.7792	58
5-isopropylnonane	0.0050	0.7842	59
2,6-dimethylheptane	0.0049	0.7891	60
cis-1-ethyl-4-methylcyclohexane	0.0049	0.7940	61
1-methyl-4-isopropylcyclohexane	0.0048	0.7988	62
4-methyloctane	0.0048	0.8037	63
trans-1-ethyl-2-methylcyclohexane	0.0048	0.8085	64
trans, cis-1,2,4-trimethylcyclohexane	0.0044	0.8129	65
trans-1,4-dimethylcyclohexane	0.0043	0.8172	66
3-methyloctane	0.0043	0.8215	67
3,5-dimethylnonane	0.0043	0.8258	68
2,4-dimethylnonane	0.0043	0.8300	69
3,3,5-trimethylheptane	0.0042	0.8343	70
cis, trans-1,2,3-trimethylcyclohexane	0.0041	0.8384	71
cis-decalinis	0.0041	0.8425	72
OTHER C12	0.0040	0.8465	73
butylcyclohexane	0.0039	0.8504	74
2,6-dimethyldecane	0.0038	0.8542	75
2-methylundecane	0.0038	0.8580	76
2,5-dimethyloctane	0.0036	0.8616	77
3-ethyl-2-methylheptane	0.0036	0.8653	78
cis, trans-1,2,4-trimethylcyclohexane	0.0036	0.8689	79
4-methylheptane	0.0036	0.8725	80
4,5-dimethyldecane	0.0036	0.8760	81
3-methylundecane	0.0032	0.8793	82
3,7-dimethyldecane	0.0032	0.8825	83
3,4-dimethyloctane	0.0032	0.8857	84
5-methylundecane	0.0032	0.8889	85
3-ethyloctane	0.0032	0.8921	86
1-ethyl-1,3-dimethylcyclohexane	0.0031	0.8952	87
cis-1-ethyl-2-methylcyclohexane	0.0031	0.8983	88
3,5-dimethyloctane	0.0030	0.9013	89
sec butylcyclohexane	0.0030	0.9043	90
2,3-dimethylheptane	0.0030	0.9073	91
4-ethyloctane	0.0029	0.9102	92
propylbenzene	0.0028	0.9130	93
OTHER C11	0.0027	0.9156	94
2,5-dimethylheptane	0.0026	0.9183	95
1-ethyl-2,4-dimethylcyclohexane	0.0026	0.9209	96
6-methylundecane	0.0026	0.9235	97
cis-decalin	0.0024	0.9259	98
1,2,3,5-tetramethylbenzene	0.0023	0.9283	99
hexylcyclopentane	0.0022	0.9304	100
2,4-dimethyldecane	0.0020	0.9324	101
2,4-dimethylheptane	0.0019	0.9343	102
1-ethyl-2,2,6-trimethylcyclohexane	0.0019	0.9362	103
OTHER C9	0.0019	0.9381	104
3-ethylhexane	0.0018	0.9399	105
trans-1-ethyl-3-methylcyclohexane	0.0018	0.9418	106
cis, cis-1,2,4-trimethylcyclohexane	0.0018	0.9436	107
butylcyclopentane	0.0018	0.9454	108
methylcyclohexane	0.0018	0.9471	109

3,4-dimethylhexane	0.0017	0.9489	110
2,7-dimethyloctane	0.0017	0.9506	111
OTHER C8	0.0017	0.9522	112
3,3,4-trimethylheptane	0.0016	0.9539	113
methyl butylcyclohexane	0.0016	0.9555	114
2,4,5-trimethylheptane	0.0016	0.9570	115
isopropylbenzene	0.0015	0.9585	116
4-methylundecane	0.0015	0.9600	117
diethylcyclohexane	0.0015	0.9615	118
2,7-dimethyldecane	0.0014	0.9629	119
1,1,3,5-tetramethylcyclohexane	0.0013	0.9642	120
1,2,4-trimethylcyclopentane	0.0013	0.9656	121
1,1-dimethyl-2-propylcyclohexane	0.0013	0.9669	122
2,4-dimethyloctane	0.0012	0.9681	123
2,3-dimethylhexane	0.0012	0.9693	124
1,1-dimethylcyclohexane	0.0012	0.9706	125
3,6-dimethyldecane	0.0012	0.9718	126
4,5-dimethylnonane	0.0012	0.9730	127
2-methyloctane	0.0012	0.9742	128
1,1,2-trimethylcyclohexane	0.0012	0.9753	129
1,2,3-trimethylcyclopentane	0.0012	0.9765	130
cis-1-ethyl-2-methylcyclopentane	0.0011	0.9776	131
3,6-dimethylnonane	0.0011	0.9788	132
3-ethylnonane	0.0011	0.9799	133
2,2,5-trimethylhexane	0.0011	0.9810	134
2,6-dimethylundecane	0.0011	0.9821	135
1,2,4-trimethylcyclohexane	0.0010	0.9831	136
2,3-dimethyloctane	0.0010	0.9841	137
cis, cis-1,3,5-trimethylcyclohexane	0.0009	0.9851	138
1-ethyl-4-isopropylbenzene	0.0009	0.9860	139
1,2,3,4-tetramethylcyclohexane	0.0009	0.9869	140
1,1,4-trimethylcyclohexane	0.0009	0.9879	141
1,2,4,5-tetramethylbenzene	0.0009	0.9887	142
2-methyldecalin	0.0009	0.9896	143
2,4-dimethylhexane	0.0008	0.9904	144
2,3,4-trimethylpentane	0.0008	0.9912	145
(2-methylbutyl)cyclohexane	0.0008	0.9920	146
methyl ethyl ketone	0.0007	0.9927	147
trans-1-ethyl-3-methylcyclopentane	0.0007	0.9933	148
4,6-dimethyldecane	0.0007	0.9940	149
methyl isobutyl ketone	0.0005	0.9946	150
5-sec butylnonane	0.0005	0.9950	151
2-ethyl-1,3-dimethylcyclohexane	0.0005	0.9955	152
cis-1,4-dimethylcyclohexane	0.0005	0.9960	153
naphthalene	0.0005	0.9965	154
4-ethyldecane	0.0005	0.9969	155
cis-1,2-dimethylcyclohexane	0.0004	0.9974	156
2,5-dimethylhexane	0.0004	0.9978	157
trans-1,2-dimethylcyclohexane	0.0004	0.9983	158
1,1,3-trimethylcyclopentane	0.0004	0.9986	159
methylcyclopentane	0.0004	0.9990	160
trans, trans-1,3,5-trimethylcyclohexane	0.0003	0.9994	161
3-ethyl-2-methylpentane	0.0003	0.9997	162
2,6-dimethylundecane	0.0003	1.0000	163

Group 10s: Solvent-based Graphic Arts Coatings			
Compound	Fraction	cum frac.	# of cmpds.
decane	0.0636	0.0636	1
1,2,4-trimethylbenzene	0.0438	0.1074	2
undecane	0.0364	0.1438	3
m-xylene	0.0345	0.1783	4
2-methylnonane	0.0330	0.2113	5
methyl propylcyclohexane	0.0329	0.2442	6
ethyl propylcyclohexane	0.0263	0.2705	7
nonane	0.0257	0.2962	8
1,3,5-trimethylbenzene	0.0241	0.3203	9
1-methyl-3-isopropylcyclohexane	0.0229	0.3432	10
1-ethyl-2-methylbenzene	0.0228	0.3660	11
2,6-dimethylnonane	0.0214	0.3875	12
propylcyclohexane	0.0212	0.4087	13
2,6-dimethyloctane	0.0211	0.4299	14
1-ethyl-4-methylbenzene	0.0194	0.4493	15
o-xylene	0.0190	0.4683	16
1,1,2,3-tetramethylcyclohexane	0.0169	0.4851	17
1-ethyl-3-methylbenzene	0.0160	0.5011	18
3-methyldecane	0.0158	0.5169	19
1,2,3-trimethylbenzene	0.0155	0.5324	20
4-methyldecane	0.0152	0.5477	21
pentylcyclopentane	0.0145	0.5622	22
2,4-dimethyloctane	0.0143	0.5764	23
cis-bicyclo[4.3.0]nonane	0.0137	0.5901	24
ethylbenzene	0.0133	0.6035	25
p-xylene	0.0133	0.6167	26
5-methyldecane	0.0129	0.6296	27
5-isopropylnonane	0.0127	0.6424	28
3,7-dimethylnonane	0.0115	0.6539	29
2,5-dimethylnonane	0.0114	0.6652	30
3-methylnonane	0.0113	0.6766	31
2-methyldecane	0.0113	0.6879	32
cis-1-ethyl-3-methylcyclohexane	0.0110	0.6988	33
isopropylcyclohexane	0.0102	0.7090	34
dodecane	0.0099	0.7190	35
methyl isopropylcyclohexane	0.0090	0.7280	36
trans-decalin	0.0088	0.7367	37
4-methylnonane	0.0087	0.7454	38
2,6-dimethyldecane	0.0086	0.7540	39
butylcyclohexane	0.0085	0.7625	40
2-ethyl-1,3-dimethylcyclohexane	0.0082	0.7707	41
4-ethylnonane	0.0080	0.7787	42
1-methyl-2-isopropylcyclohexane	0.0079	0.7866	43
propylbenzene	0.0075	0.7941	44
isobutylcyclohexane	0.0072	0.8013	45
OTHER C11	0.0071	0.8084	46
2-methyldecalin	0.0069	0.8153	47
3,5-dimethyloctane	0.0068	0.8221	48
1,3-dimethyl-2-isopropylcyclopentane	0.0066	0.8287	49
OTHER C10	0.0063	0.8350	50
3,5-dimethylnonane	0.0062	0.8412	51
OTHER C12	0.0062	0.8474	52
3,6-dimethyloctane	0.0056	0.8530	53
1-ethyl-1,3-dimethylcyclohexane	0.0055	0.8585	54
3,4-dimethyloctane	0.0054	0.8639	55
1,3-dimethyl-5-ethylbenzene	0.0052	0.8691	56
trans, cis-1,2,4-trimethylcyclohexane	0.0051	0.8742	57
cis-1-ethyl-2-methylcyclohexane	0.0051	0.8793	58
pentylcyclohexane	0.0049	0.8843	59
diethylcyclohexane	0.0048	0.8890	60
5-methylindane	0.0047	0.8937	61
hexylcyclopentane	0.0047	0.8984	62
6-methylundecane	0.0047	0.9030	63
trans-1-ethyl-3-methylcyclohexane	0.0041	0.9071	64
cis-1-ethyl-4-methylcyclohexane	0.0040	0.9111	65
1,1-dimethyl-2-propylcyclohexane	0.0039	0.9150	66
OTHER C9	0.0038	0.9189	67
2-methylundecane	0.0038	0.9227	68
cis, trans-1,2,3-trimethylcyclohexane	0.0038	0.9265	69
1,2,3-trimethylcyclohexane	0.0038	0.9302	70
indane	0.0034	0.9336	71
cis-decalin	0.0031	0.9368	72
2-methyloctane	0.0030	0.9398	73
3-methylundecane	0.0030	0.9428	74
cis, trans-1,2,4-trimethylcyclohexane	0.0029	0.9457	75
trans-1-ethyl-2-methylcyclohexane	0.0029	0.9486	76
trans, trans-1,3,5-trimethylcyclohexane	0.0028	0.9514	77
4-methylundecane	0.0028	0.9542	78
1,2-diethyl-1-methylcyclohexane	0.0028	0.9570	79
3,3,5-trimethylheptane	0.0027	0.9597	80
3-methyloctane	0.0025	0.9622	81
trans-1-ethyl-4-methylcyclohexane	0.0025	0.9647	82
1,3-diethylbenzene	0.0024	0.9671	83
1-ethyl-1,2-dimethylcyclohexane	0.0022	0.9693	84
isopropylbenzene	0.0022	0.9715	85
3-ethyl-4-methylheptane	0.0020	0.9735	86
1,1,3-trimethylcyclohexane	0.0017	0.9752	87
(2-methylbutyl)cyclohexane	0.0016	0.9769	88
cis, cis-1,2,4-trimethylcyclohexane	0.0016	0.9784	89
2,5-dimethyloctane	0.0015	0.9799	90
2,4-dimethylnonane	0.0015	0.9814	91
3-ethyloctane	0.0014	0.9828	92
2,6-dimethylundecane	0.0014	0.9843	93
2,3-dimethylheptane	0.0013	0.9856	94
trans, trans-1,2,4-trimethylcyclohexane	0.0013	0.9869	95
2,4-dimethyldecane	0.0012	0.9881	96
1,3-dimethyl-2-ethylbenzene	0.0012	0.9893	97
3,4-dimethylhexane	0.0012	0.9905	98
toluene	0.0011	0.9916	99
naphthalene	0.0009	0.9925	100
5-methylundecane	0.0009	0.9934	101
2,6-dimethylheptane	0.0008	0.9942	102
3-methylpentane	0.0008	0.9950	103
octane	0.0007	0.9957	104
5,6-dimethylindane	0.0007	0.9964	105
1,1,4-trimethylcyclohexane	0.0006	0.9969	106
ethylcyclohexane	0.0006	0.9975	107

2,5-dimethylheptane	0.0005	0.9980	108
1,1-dimethylcyclohexane	0.0005	0.9985	109
cis-1,3-dimethylcyclohexane	0.0004	0.9989	110
3-ethyldecane	0.0004	0.9994	111
cis-1,4-dimethylcyclohexane	0.0004	0.9997	112
4-methylheptane	0.0003	1.0000	113

Group 11s: Thinning Solvents			
Compound	Fraction	cum frac.	# of cmpds.
methylcyclohexane	0.0980	0.0980	1
heptane	0.0510	0.1490	2
undecane	0.0447	0.1937	3
decane	0.0434	0.2371	4
toluene	0.0415	0.2786	5
octane	0.0386	0.3171	6
acetone	0.0348	0.3519	7
cis-1,3-dimethylcyclohexane	0.0246	0.3765	8
ethanol	0.0237	0.4002	9
2-methylheptane	0.0218	0.4220	10
2,6-dimethylnonane	0.0140	0.4359	11
1,2,4-trimethylbenzene	0.0138	0.4498	12
3-methylheptane	0.0138	0.4636	13
1,2,4-trimethylcyclopentane	0.0133	0.4769	14
2-methylhexane	0.0129	0.4898	15
trans, trans-1,2,4-trimethylcyclohexane	0.0121	0.5019	16
nonane	0.0117	0.5136	17
1,2-dimethylcyclopentane	0.0115	0.5252	18
butyl acetate	0.0114	0.5366	19
m-xylene	0.0112	0.5478	20
ethyl propylcyclohexane	0.0110	0.5587	21
ethylcyclohexane	0.0101	0.5689	22
4-methylnonane	0.0094	0.5783	23
methyl amyl ketone	0.0086	0.5869	24
trans-1,4-dimethylcyclohexane	0.0085	0.5954	25
trans-1,3-dimethylcyclohexane	0.0083	0.6038	26
2-methyldecane	0.0083	0.6120	27
methyl propylcyclohexane	0.0082	0.6202	28
2,6-dimethylheptane	0.0076	0.6279	29
3-methyldecane	0.0075	0.6354	30
cis, cis-1,3,5-trimethylcyclohexane	0.0069	0.6423	31
1,2,3-trimethylcyclopentane	0.0068	0.6492	32
trans, cis-1,2,4-trimethylcyclohexane	0.0067	0.6558	33
1,1,3-trimethylcyclopentane	0.0066	0.6624	34
1,1,3-trimethylcyclohexane	0.0065	0.6690	35
4-methyldecane	0.0064	0.6753	36
trans, trans-1,3,5-trimethylcyclohexane	0.0063	0.6817	37
5-methyldecane	0.0063	0.6880	38
1,2,3-trimethylbenzene	0.0063	0.6943	39
4-methylheptane	0.0060	0.7003	40
butylcyclohexane	0.0058	0.7061	41
dodecane	0.0057	0.7118	42
2-methylnonane	0.0056	0.7174	43
ethylcyclopentane	0.0056	0.7230	44
trans-1,3-dimethylcyclopentane	0.0054	0.7284	45
2,6-dimethyloctane	0.0054	0.7338	46
5-methylindane	0.0052	0.7390	47
1-methyl-4-propylbenzene	0.0051	0.7442	48
2-butoxyethanol	0.0048	0.7489	49
2,4-dimethylhexane	0.0045	0.7534	50
1-ethyl-4-methylbenzene	0.0045	0.7579	51
4-methyloctane	0.0045	0.7623	52
2,5-dimethylheptane	0.0044	0.7668	53
cis-1-ethyl-3-methylcyclohexane	0.0044	0.7712	54
3,7-dimethylnonane	0.0044	0.7755	55
ethylbenzene	0.0043	0.7799	56
propylcyclohexane	0.0043	0.7842	57
1-methyl-3-isopropylbenzene	0.0041	0.7883	58
cis-1,3-dimethylcyclopentane	0.0041	0.7924	59
1-methylindane	0.0041	0.7964	60
3-methyloctane	0.0040	0.8004	61
1,2,3-trimethylcyclohexane	0.0040	0.8044	62
OTHER C12	0.0039	0.8083	63
2,5-dimethylnonane	0.0037	0.8120	64
methanol	0.0037	0.8157	65
1-ethyl-2-methylbenzene	0.0037	0.8193	66
p-xylene	0.0035	0.8228	67
1-methyl-3-isopropylcyclohexane	0.0035	0.8263	68
2,3-dimethyloctan	0.0034	0.8297	69
1,2-dimethyl-4-ethylbenzene	0.0034	0.8331	70
3-methylnonane	0.0033	0.8364	71
1-ethyl-3-methylbenzene	0.0033	0.8397	72
o-xylene	0.0032	0.8429	73
pentylcyclopentane	0.0032	0.8461	74
3-ethylhexane	0.0032	0.8493	75
1-methyl-2-isopropylcyclohexane	0.0032	0.8525	76
2,3-dimethylhexane	0.0032	0.8557	77
2-methyloctane	0.0031	0.8588	78
OTHER C9	0.0030	0.8618	79
isobutylcyclohexane	0.0030	0.8648	80
2-methylundecane	0.0030	0.8678	81
1,2,3,5-tetramethylbenzene	0.0029	0.8706	82
isopropylcyclohexane	0.0029	0.8735	83
cis, trans-1,2,4-trimethylcyclohexane	0.0028	0.8763	84
1,1-dimethylcyclohexane	0.0026	0.8789	85
1,3-dimethyl-2-ethylbenzene	0.0026	0.8815	86
2,6-dimethyldecane	0.0026	0.8841	87
1,3-dimethyl-5-ethylbenzene	0.0026	0.8866	88
naphthalene	0.0025	0.8891	89
diethylcyclohexane	0.0024	0.8915	90
2,4-dimethylheptane	0.0023	0.8938	91
trans-1-ethyl-3-methylcyclohexane	0.0023	0.8961	92
1,2,4,5-tetramethylbenzene	0.0022	0.8983	93
1,1,2-trimethylcyclopentane	0.0022	0.9005	94
pentylcyclohexane	0.0021	0.9026	95
1,4-dimethyl-2-ethylbenzene	0.0021	0.9047	96
trans-1-ethyl-4-methylcyclohexane	0.0021	0.9067	97
1-methyl-3-propylbenzene	0.0020	0.9088	98
indane	0.0020	0.9108	99
3-ethyl-2-methylheptane	0.0019	0.9127	100
4,5-dimethyloctane	0.0019	0.9145	101
1,1,3,4-tetramethylcyclohexane	0.0018	0.9164	102
6-methylundecane	0.0018	0.9182	103
3-phenylpentane	0.0018	0.9201	104
6-ethyl-2-methyloctane	0.0018	0.9218	105
1-ethyl-3-methylcyclopentane	0.0017	0.9236	106
2,3-dimethylpentane	0.0017	0.9253	107
1,2-dimethyl-3-ethylcyclohexane	0.0017	0.9270	108
1-ethyl-2-methylcyclopentane	0.0017	0.9287	109
3-ethylheptane	0.0016	0.9303	110
cis-1,4-dimethylcyclohexane	0.0016	0.9320	111
cyclohexane	0.0016	0.9336	112
OTHER C10	0.0016	0.9352	113
4-ethyldecane	0.0016	0.9368	114
3-methylhexane	0.0015	0.9384	115

1-ethyl-4-isopropylbenzene	0.0015	0.9399	116
cis-bicyclo[4.3.0]nonane	0.0015	0.9414	117
3,4-dimethylhexane	0.0015	0.9429	118
1,1,4-trimethylcyclohexane	0.0015	0.9444	119
2,3-dimethyloctane	0.0015	0.9458	120
3-ethyl-3-methyloctane	0.0014	0.9473	121
2-methyldecalin	0.0014	0.9487	122
OTHER C11	0.0014	0.9501	123
1,3-dimethyl-4-ethylbenzene	0.0014	0.9514	124
trans-1-ethyl-2-methylcyclohexane	0.0013	0.9527	125
cis, cis-1,2,4-trimethylcyclohexane	0.0013	0.9541	126
3-methylundecane	0.0013	0.9554	127
1,2-diethyl-1-methylcyclohexane	0.0013	0.9566	128
(2-methylbutyl)cyclohexane	0.0013	0.9579	129
3,6-dimethyloctane	0.0013	0.9591	130
4-methylundecane	0.0012	0.9604	131
2,2,5-trimethylhexane	0.0012	0.9616	132
3,5-dimethyloctane	0.0012	0.9628	133
1,3,5-trimethylbenzene	0.0012	0.9639	134
5-methylundecane	0.0011	0.9651	135
hexylcyclopentane	0.0011	0.9662	136
3,4-dimethyloctane	0.0011	0.9673	137
3-ethyloctane	0.0011	0.9684	138
2-ethyl-1,3-dimethylcyclohexane	0.0011	0.9695	139
sec butylbenzene	0.0011	0.9705	140
5-isopropylnonane	0.0011	0.9716	141
1,1-dimethylcyclopentane	0.0010	0.9725	142
cis-1,2-dimethylcyclohexane	0.0010	0.9735	143
cis, trans-1,2,3-trimethylcyclohexane	0.0009	0.9744	144
2,3,4-trimethylpentane	0.0009	0.9754	145
4-methylindane	0.0009	0.9763	146
2,6-dimethylundecane	0.0009	0.9772	147
3-ethyl-2-methylpentane	0.0008	0.9780	148
propylcyclopentane	0.0008	0.9788	149
1-ethyl-2,2,6-trimethylcyclohexane	0.0008	0.9796	150
2,4-dimethylpentane	0.0008	0.9803	151
2,7-dimethyloctane	0.0008	0.9811	152
1,1-dimethyl-2-propylcyclohexane	0.0008	0.9818	153
trans-1,2-dimethylcyclohexane	0.0007	0.9826	154
1,1,2-trimethylcyclohexane	0.0007	0.9833	155
1-ethyl-1-methylcyclopentane	0.0007	0.9839	156
1-ethyl-1,2-dimethylcyclohexane	0.0007	0.9846	157
1-methyl-4-isobutylbenzene	0.0006	0.9852	158
3,3,5-trimethylheptane	0.0006	0.9858	159
cis-decalin	0.0006	0.9864	160
1,1,2,3-tetramethylcyclohexane	0.0006	0.9870	161
2,4-dimethylnonane	0.0006	0.9876	162
1-ethyl-2,4-dimethylcyclohexane	0.0006	0.9881	163
1-methyl-4-isopropylbenzene	0.0005	0.9886	164
3-ethyldecane	0.0005	0.9892	165
cis-1-ethyl-2-methylcyclohexane	0.0005	0.9897	166
tridecane	0.0005	0.9902	167
cis-bicyclo[3.3.0]octane	0.0005	0.9907	168
cis-1-ethyl-4-methylcyclohexane	0.0005	0.9912	169
1,3-dimethyl-4-isopropylbenzene	0.0005	0.9917	170
propylbenzene	0.0005	0.9921	171
4,5-dimethyldecane	0.0005	0.9926	172
2,2,3,3-tetramethylpentane	0.0004	0.9930	173
2-methylnaphthalene	0.0004	0.9934	174
isopropylbenzene	0.0004	0.9938	175
cis-1-ethyl-2-methylcyclopentane	0.0004	0.9942	176
OTHER C13	0.0004	0.9946	177
OTHER OTHER C8	0.0003	0.9949	178
2,7-dimethyldecane	0.0003	0.9953	179
3,5-dimethylnonane	0.0003	0.9956	180
2,5-dimethylhexane	0.0003	0.9959	181
2,2-dimethylheptane	0.0003	0.9962	182
1-methyl-3-butylbenzene	0.0003	0.9964	183
methyl isobutyl ketone	0.0003	0.9967	184
2,3-dimethylheptane	0.0003	0.9969	185
2,3,5-trimethylheptane	0.0002	0.9972	186
2,5-dimethyloctane	0.0002	0.9974	187
butyl alcohol	0.0002	0.9976	188
1,2,3-trimethyl-4-ethylbenzene	0.0002	0.9978	189
1,1,3,5-tetramethylcyclohexane	0.0002	0.9981	190
cis-1-ethyl-3-methylcyclopentane	0.0002	0.9983	191
3-ethyl-4-methylheptane	0.0002	0.9985	192
trans-1-ethyl-3-methylcyclopentane	0.0002	0.9987	193
hexylcyclohexane	0.0002	0.9988	194
OTHER C14	0.0002	0.9990	195
styrene	0.0002	0.9992	196
1-methyl-4-isopropylcyclohexane	0.0001	0.9993	197
2,4-dimethyloctane	0.0001	0.9994	198
methyl pentylcyclohexane	0.0001	0.9996	199
methyl ethyl ketone	0.0001	0.9997	200
3-ethyl-2methylpentane	0.0001	0.9998	201
methylcyclopentane	0.0001	0.9999	202
OTHER C7	0.0000	1.0000	203
2-methylbutane	0.0000	1.0000	204