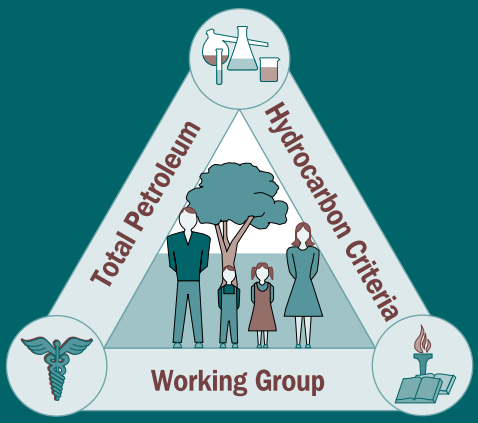
Total Petroleum Hydrocarbon Criteria Working Group Series

Volume 2

Composition of Petroleum Mixtures



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Composition of Petroleum Mixtures

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Composition of Petroleum Mixtures

MAY 1998

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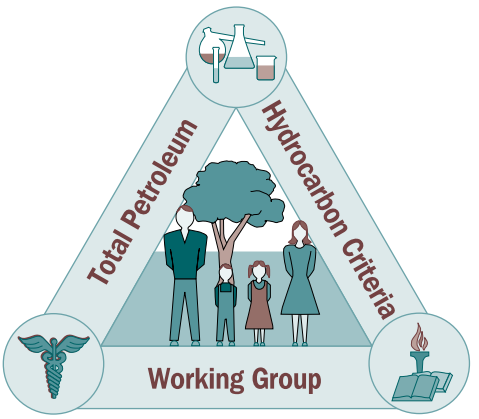

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FOREWORD

This document is second in a series from the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG, or "Working Group"). The Working Group convened in 1993 to address the large disparity among cleanup requirements being used by states at sites contaminated with hydrocarbon materials such as fuels, lubricating oils and crude oils. These requirements usually focus on total petroleum hydrocarbon (TPH), with numerical standards ranging from tens to tens of thousands of milligrams of TPH per kilogram of soil. Recognizing that these standards are not based on a scientific assessment of human health risk, Working Group members established the following goal for their effort:

To develop scientifically defensible information for establishing soil cleanup levels that are protective of human health at petroleum contaminated sites.

The Working Group is guided by a steering committee consisting of representatives from industry, government, and academia. Some of the active participants, among the more than 400 involved, include: the Gas Research Institute, several major petroleum companies (Chevron, Exxon, British Petroleum and Shell), the American Petroleum Institute, the Association of American Railroads, several state governments (Washington, Texas, Colorado, Hawaii, Louisiana, New Mexico, Massachusetts), the U.S. Environmental Protection Agency, the Department of Defense, the University of Massachusetts, and private consulting firms including EA Engineering, Science & Technology, and Menzie-Cura & Associates, Inc.

The Working Group compiled their data collection and analytical efforts into five volumes:

Volume 1. Analysis of Petroleum Hydrocarbons in Environmental Media discusses and critiques analytical methods for quantifying TPH, petroleum mixtures and individual petroleum constituents in soil and water samples. It is designed to be a reference tool for the nonchemist, describing what information analytical methods can provide for risk assessment.

Volume 2. Composition of Petroleum Mixtures provides the best available composition information for a variety of petroleum products.

Volume 3. Selection of Representative Total Petroleum Hydrocarbon (TPH) Fractions Based on Fate and Transport Considerations defines fractions of TPH expected to behave similarly in the environment. Identification of these fractions simplifies analysis of environmental samples, fate and transport modeling, and risk assessment efforts at petroleum contaminated sites.

Volume 4. Development of Fraction-Specific Reference Doses (RfDs) and Reference Concentrations (RfCs) for Total Petroleum Hydrocarbons (TPH). This volume provides the technical basis for the development of TPH fraction-specific RfDs and RfCs for use in the hazard

assessment step of the Working Group's risk-based approach to establishing soil cleanup levels at petroleum contaminated sites.

Volume 5. Human Health Risk-Based Evaluation of Petroleum Contaminated Sites: Implementation of the Working Group Approach. This volume integrates the findings of Volumes 1 through 4 into a risk-based framework for development of cleanup goals at petroleum contaminated sites. It includes descriptions of demonstration sites where the Working Group method has been used successfully.

Amherst Scientific Publishers will publish these volumes in 1997 and 1998. In addition to these volumes, results of projects where use of the Working Group approach has been demonstrated (demonstration sites) and a concise technical summary document are now or will soon be available on the U.S. Air Force Research Laboratory, Operational Toxicology Branch web site (http://voyager.wpafb.af.mil). At this web site, Working Group publications may be downloaded from the "recent publications" icon. Additional Working Group resources will be added to this web site as they become available.

We hope you find these documents to be useful in your effort to evaluate and determine acceptable risk-based cleanup criteria at petroleum contaminated sites.

Wade H. Weisman
Chairman, TPH Criteria Working Group

ACKNOWLEDGMENTS

The publication of this volume of the Total Petroleum Hydrocarbon Criteria Working Group Series would not have been possible without the hard work and dedication of individuals across public and private sectors. The comprehensive petroleum fuel mixtures database presented in this document was crucial to the Working Group's delineation of fate and transport fractions and corresponding toxicity criteria. We would specifically like to acknowledge the following individuals for their efforts in the completion of this volume:

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1.0 INTRODUCTION

Risk-based analysis of petroleum contaminated soil is hampered by the lack of readily available data describing the composition of common petroleum products and crude oil. There is not one governmental agency, industry or group which compiles the data in a manner necessary to assess the risks posed by the hydrocarbon constituents. Composition data are rare for several reasons. Crude oil and its products are highly complex and variable mixtures. Consequently, constituent-specific chemical analysis of these mixtures is challenging. In addition, the data necessary for risk analysis are often much more detailed than that required by the petroleum industry for determining the performance characteristics of petroleum mixtures.

In the absence of these data, assumptions regarding composition are made which may be incorrect or misleading. Often assumptions are very conservative and do not take into account the impacts of weathering. Once petroleum hydrocarbon mixtures are released into the environment, their composition changes due to processes such as biodegradation, dissolution in water and volatilization. Taken together these processes are termed weathering. Each is selective for specific hydrocarbon groups. Generally mixtures become less water-soluble and less volatile as they weather. These changes are functions of the rate at which the more soluble and volatile constituents leach or evaporate from soil. A more detailed discussion of weathering is provided in section 3.3 of this document.

To advance risk-based analysis of petroleum contaminated soils, a comprehensive search of the technical literature was performed to identify all available composition data for the most common petroleum-based fuels, crude oil and lubricating oils. The data are compiled in a uniform format in this document. A brief discussion is provided of petroleum hydrocarbon chemistry, how weathering influences the chemistry of products after release to the environment, and petroleum composition research needs.

2.0 PETROLEUM CHEMISTRY

Crude oil, the source material of nearly all petroleum products, contains a wide variety of elements combined in various forms.[1] The principal constituents are carbon and hydrogen which in their combined form are hydrocarbons. In the refining process petroleum products are strongly enriched with hydrocarbons, leaving most crude-based inorganic materials and other types of organic compounds containing sulfur, nitrogen and oxygen in the residual material.

2.1 GENERAL PETROLEUM CHEMISTRY

Petroleum hydrocarbons are organic compounds comprised of carbon and hydrogen atoms arranged in varying structural configurations. In the broadest sense, they are divided into two families, *aliphatics* (fatty) and *aromatics* (fragrant). Aliphatics are further divided into three main classes, *alkanes*, *alkenes* and *cycloalkanes*. Figure 1 illustrates hydrocarbon structural relationships. Alkynes, another type of aliphatic structure, are not commonly found in petroleum hydrocarbons. They are not discussed further in this document.

On a molecular level, aliphatic and aromatic compounds differ by the patterns of bonding between adjacent carbon atoms. Aromatic molecules have ring structures and are basically flat and symmetric with clouds of electrons above and below the plane of the molecule. Aromatic carbon-carbon bonds are termed resonance bonds in that electrons are shared between multiple carbon atoms. In this sense the electrons are "delocalized" (participating in several bonds). This imparts chemical stability. Highly directional bonds, in which carbon atoms share electrons only with adjacent carbons, are characteristic of aliphatic structures. The molecules are essentially free to rotate around these bonds, thus the aliphatic structures can assume many different conformations.

The bonding pattern of aromatic structures contributes to their moderate polarity. The electron clouds surrounding the molecules can be deformed by the charge on adjacent molecules. This results in the development of partial positive and negative charge sites on the molecule. This is in contrast to the aliphatics that are nonpolar or only slightly polar. Their bonding pattern does not permit nonuniform distribution of charge to the same degree.

The polarity of hydrocarbon structures governs the degree to which molecules interact with themselves and with water. Generally, as polarity increases, water solubility (i.e. interaction with water) and boiling points increase. It follows that aromatics are more water soluble and less volatile than alkanes with a corresponding number of carbons.

Within each hydrocarbon structural family and sub-family, there are *homologous series*. Each member of the series is termed a *homolog* and differs from adjacent members in the series by a repeating unit such as a CH_2 group. Within a homologous series, physical properties of compounds change with the number of carbon atoms. For example, there is an increase in the boiling point of approximately 20°C for each carbon atom added to an *n*-alkane chain. Generally, the persistence of petroleum hydrocarbon compounds in the environment increases with an increase in the compound's boiling point.

Another key feature of petroleum hydrocarbons is that they typically have a large number of *isomers*. Isomers are compounds that have the same elemental formula but have different structural configurations. Different types of isomers are described in the sections below. In general, as the carbon number increases, the number of possible isomers increases rapidly. An alkane with six carbon atoms has five possible isomers. Increasing the number of carbons to ten increases the number of possible isomers to seventy-five. The large number of isomeric compounds in petroleum mixtures accounts for their high degree of complexity. Petroleum mixtures with high boiling point constituents have high average carbon numbers; therefore, they have a large number of isomers and greater chemical complexity than petroleum products with low boiling point constituents.

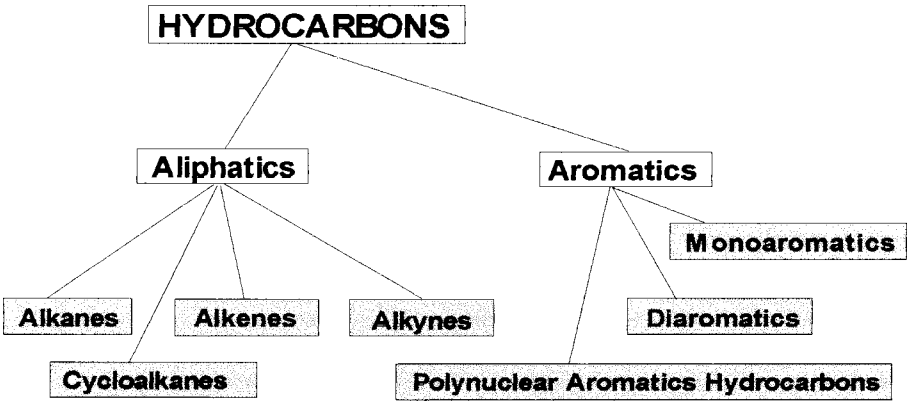
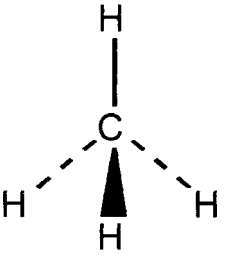


Figure 1. Hydrocarbon Structural Relationships

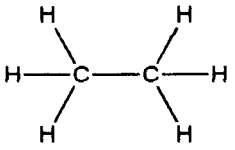
2.2 ALKANES

Within the aliphatic structure classification (see Figure 1), there are alkanes, alkenes, and cycloalkanes. Alkanes contain only single carbon-carbon bonds. The simplest alkane structure is methane (CH_4), which is comprised of a single carbon atom and four hydrogen atoms (Figure 2). Methane is the single carbon *homolog* (member of a structural series), and ethane is the two-carbon homolog in the *straight-chain* alkane family. Ethane (C_2H_6) consists of two carbon atoms, each of which participates in directional bonds with three hydrogen atoms and the other carbon atom. The homologous series of straight-chain alkanes continues with propane (C_3H_8), butane (C_4H_{10}), pentane (C_5H_{12}) and so on (see Figure 3 and Table 1), where carbons are attached to no more than two other carbons in a continuous chain, and the chains have two methyl (-CH_3) terminations. These alkanes are given an *n-* prefix to designate the straight-chain structural configuration. So "*n*-pentane" is a straight-chain alkane with five carbons and twelve hydrogens (C_5H_{12}) .

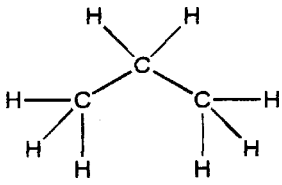


methane

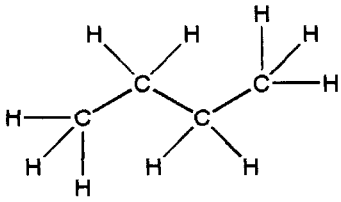
Figure 2. This structural representation of methane shows the carbon atom at the center of a tetrahedron, with the four hydrogen atoms at the corners. The bond represented by a solid line, lies in, those represented by dashed lines go away from, and that represented by a filled triangle comes out of the plane of the page.



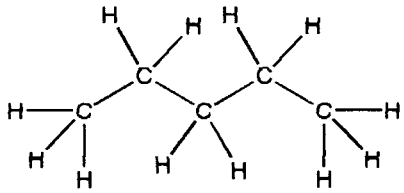
ethane



propane



n-butane



n-pentane

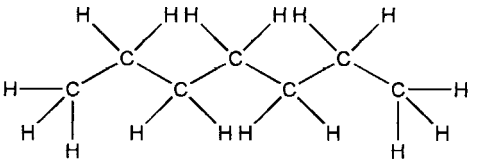
Figure 3. Structures for the Homologous Series of Ethane, Propane, *n*-Butane and *n*-Pentane

Table 1. Alkane Nomenclature and Chemical Formulas

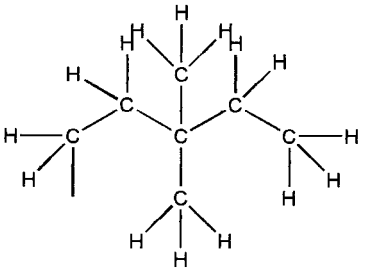
Name	Formula	Name	Formula
methane	CH_4	heneicosane	$C_{21}H_{44}$
ethane	C_2H_6	docosane	$C_{22}H_{46}$
propane	C_3H_8	tricosane	$C_{23}H_{48}$
butane	C_4H_{10}	tetracosane	$C_{24}H_{50}$
pentane	C_5H_{12}	pentacosane	$C_{25}H_{52}$
hexane	C_6H_{14}	hexacosane	$C_{26}H_{54}$
heptane	C_7H_{16}	heptacosane	$C_{27}H_{56}$
octane	C_8H_{18}	octacosane	$C_{28}H_{58}$
nonane	C_9H_{20}	nonacosane	$C_{29}H_{60}$
decane	$C_{10}H_{22}$	triacontane	$C_{30}H_{62}$
undecane	$C_{11}H_{24}$	hentricontane	$C_{31}H_{64}$
dodecane	$C_{12}H_{26}$	dotriacontane	$C_{32}H_{66}$
tridecane	$C_{13}H_{28}$	tritriacontane	$C_{33}H_{68}$
tetradecane	$C_{14}H_{30}$	tetratriacontane	$C_{34}H_{70}$
pentadecane	$C_{15}H_{32}$	pentatriacontane	$C_{35}H_{72}$
hexadecane	$C_{16}H_{34}$	hexatiacontane	$C_{36}H_{74}$
heptadecane	$C_{17}H_{36}$	heptatriacontane	$C_{37}H_{76}$
octadecane	$C_{18}H_{38}$	octatriacontane	$C_{38}H_{78}$
nonadecane	$C_{19}H_{40}$	nonatriacontane	$C_{39}H_{80}$
eicosane	$C_{20}H_{42}$	tetracontane	$C_{40}H_{82}$

Alkane groups that are substituted onto hydrocarbon structures have their carbon numbers described by the same prefixes of Table 1, and the complete nomenclature has a *-yl* suffix. So a single-carbon alkyl substituent is named *methyl-* , the two-carbon substituent is named *ethyl-* , the three-carbon substituent is named *propyl-* , and so on.

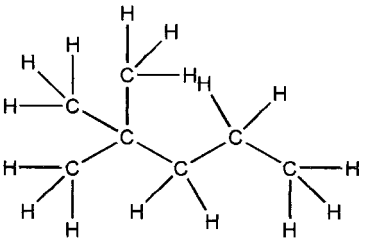
Str uctural isomers are compounds that share a chemical formula, but have distinct chemical structures. *n*-Heptane, 3,3-dimethylpentane and isoheptane are all described by C_7H_{16}, but their structures are very different (see Figure 4). *n*-Heptane describes a straight-chain alkane, whereas 3,3-dimethylpentane and isoheptane describe *branched alkanes*. 3,3-Dimethylpentane has two methyl groups attached to the third atom of an *n*-pentane chain. Isoheptane has three terminal methyl groups on one end of an *n*-pentane structure. The *iso* prefix denotes a branched-chain alkane with three terminal methyl groups on one end of a straight-chain structure.



n-heptane



3,3-dimethylpentane



isoheptane

Figure 4. The Structural Isomers *n*-Heptane, 3,3-Dimethylpentane and Isoheptane

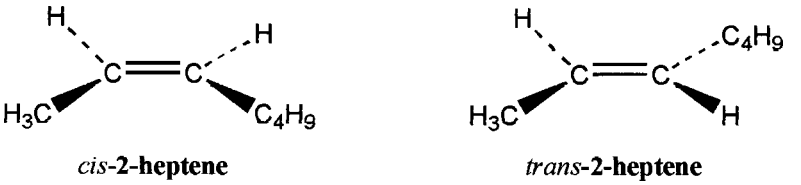
2.3 ALKENES

Alkenes are hydrocarbons that contain less hydrogen, carbon for carbon, than the corresponding alkane. This is due to the occurrence of one or more double bonds between carbon atoms in the alkene structure. An alkene is the *unsaturated* form of the corresponding *saturated* alkane. Butene is described by the chemical formula C_4H_8, whereas butane, the corresponding alkane structure, is described by C_4H_{10}. Alkenes are named by replacing the ending *-ane* of the corresponding alkane name (Table 1) with *-ene.* The alkene name is preceded by a number (or numbers in the case of multiple double bonds) that indicates the position of the first double-bonded carbon encountered in the chain. 2-Pentene describes a hydrocarbon that is a five-membered chain with a double bond between the second and third carbons.

Alkenes that contain two double bonds are termed *dienes* . When the two double bonds are separated by one single bond, they become *conjugated* dienes. Conjugated dienes exhibit increased stability because of the fact that the electrons are delocalized across the two double bonds and the single bond between them. The electron pair of any conjugated double bond is not centered over a singular double bond. Rather, the electron pair density is distributed around the entire diene group so that the carbon-to-carbon bonds can be thought of as partially single bonds and partially double bonds.

A carbon atom involved in a double bond lies at the center of a flat triangle, with the three bonds being directed toward the triangle corners. The two carbon atoms of a

double bond and the four groups attached to them all lie within the same plane. The structural configuration of the double bond gives rise to *geometric isomers* when one of the substituent groups on each of the two double-bonded carbons is not simply hydrogen. For example, 2-heptene describes two geometric isomers that are further described as *cis* -2-heptene and *trans* -2-heptene (see Figure 5). With reference to the hydrogen atoms attached to the carbons in the double bond, *cis* -2-heptene has its hydrogens situated on the same side of the double bond, and *trans* -2-heptene has its hydrogen groups on opposing sides of the double bond.

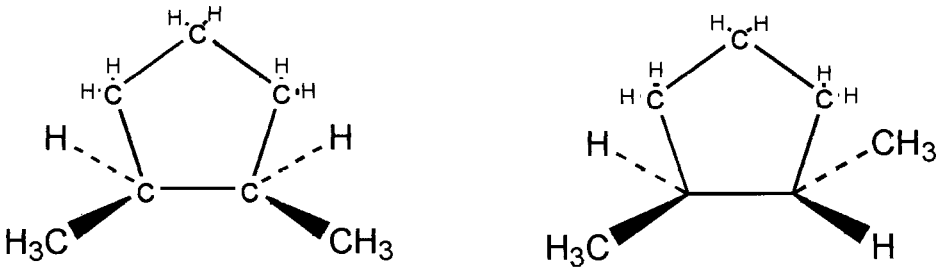


cis-**2-heptene** *trans*-**2-heptene**

Figure 5. The Geometric Isomers *cis*-2-Heptene and *trans*-2-Heptene

2.4 CYCLOALKANES

Cycloalkanes are alkanes where carbon atoms form cyclic structures. The naming of cycloalkanes is the same as the naming of alkanes (see Table 1) with the addition of a *cyclo* - prefix. So a five-carbon alkane ring is cyclopentane. Cycloalkane compounds can exhibit *configurational isomerism* in that attached groups can differ in their positions relative to the ring. The cycloalkane prefix of *cis* - denotes that two groups (other than hydrogen) attached to the ring both lie either above or below the plane of the ring. *Trans* - denotes that one of the two groups, lies above and the other lies below the plane of the ring. In the molecule *cis* -1,2-dimethylcyclopentane, there are two methyl groups attached to the first and second carbon of a five-carbon ring, and the attached groups both lie either above or below the plane of the five-carbon ring (see Figure 6). By contrast, *trans* - 1,2-dimethylcyclopentane has one of the two attached methyl groups positioned above, and the other positioned below, the plane of the ring.



cis-**1,2-dimethylcyclopentane** *trans*-**1,2-dimethylcyclopentane**

Figure 6. The Configurational Isomers *cis*- and *trans*-1,2-Dimethylcyclopentane

2.5 AROMATICS

Aromatic hydrocarbons have one or more benzene rings as structural components. Benzene is a six-membered carbon ring with the chemical formula C_6H_6. There are three carbon-to-carbon single bonds that alternate with three carbon-to-carbon double bonds. The bonds of benzene have electron pairs that are delocalized across the entire six-membered ring. This gives benzene more "polar" characteristics than alkanes or alkenes, since its electron clouds are easily deformed by opposite charges on other molecules.

A *monoar omatic* compound has one benzene ring with either six hydrogen groups, or a combination of alkyl and hydrogen groups, attached to that six-carbon aromatic ring (see Figure 7). A *diaromatic* compound has two fused benzene rings as its basis with eight hydrogen or alkyl groups attached to the rings. The electron pairs of the five double bonds are delocalized across both rings of the diaromatics. *Polynuclear ar omatic hydr ocarbons (P AHs)* have more than two fused benzene rings as a structural characteristic, and their structural stability results from the concomitant electron pair delocalization. PAHs can have various alkyl groups and hydrogens attached to the multi-ringed structure. In general, alkyl-substituted PAHs predominate in petroleum. For example, there are much higher concentrations of methylphenanthrene and dimethylphenanthrene in diesel fuel than phenanthrene.

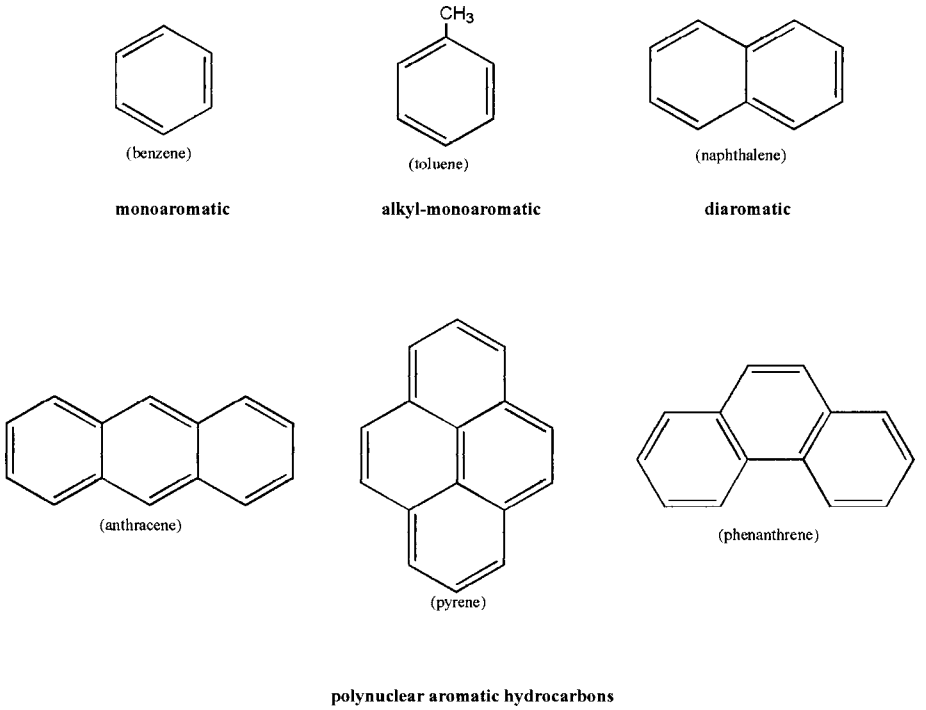


Figure 7. Structures of a Monoaromatic, an Alkyl-monoaromatic, a Diaromatic and Polynuclear Aromatic Hydrocarbons

2.6 OTHER PETROLEUM FUEL MIXTURE COMPONENTS

Organic compounds containing sulfur, nitrogen and oxygen may be encountered at significant concentrations in crude oil and in some heavier fuels such as No.6 fuel oil. Sulfur-containing heterocyclic aromatic compounds are the major constituents. They are mainly in the form of thiophenes and thiophene derivatives. Nitrogen heterocyclics are present as derivatives of thiazole and quinoline, although they are present at much lower concentrations than the sulfur derivatives.

Metals are also encountered in petroleum fuel mixtures in the form of salts of carboxylic acids, or as porphyrin chelates.[2] Vanadium and nickel are predominant occurring at highest concentration in crude oil and residual fuel oils.

3.0 PETROLEUM FUEL MIXTURE PRODUCTION

3.1 PETROLEUM REFINING PROCESS

Petroleum fuel mixtures are produced from crude oil through a variety of refining and blending processes.[3] After treatment to remove dissolved gas, dirt and water, crude oil is distilled and a variety of petroleum product fractions results. The fractions can be used directly or their hydrocarbon composition can be altered through *cracking* and/or *refor ming*. Cracking is a process that converts long-chain alkanes into smaller alkanes, alkenes, and some hydrogen. It is this process which accounts for the occurrence of alkenes in petroleum fuel mixtures. Alkenes are not abundant in crude oil. Reforming is a process that converts aliphatics into aromatics. Composition of a distillation fraction can also be altered through *treatment* . Treatment can involve removal or conversion of undesirable components, or addition of desired components. The products of the refining process are blended to yield petroleum fuel mixtures with characteristics required for desired end uses. Blending agents and additives used for various petroleum fuel mixtures are shown in Table 2.[4] Of these, only lead, barium, methyl-*ter t*-butylether (MTBE), and ethylene dibromide (EDB) are likely to be detected in environmental samples. Analytical methods for these substances are well-developed and are routinely performed in environmental laboratories.

Table 2. Types of Blending Agents and Additives for Petroleum Fuel Mixtures

Petroleum Fuel Mixture	Type	Compounds
Gasoline	anti-knock	2,2,4-trimethylpentane
		tetraethyl lead
		tetramethyl lead
		tert-butyl alcohol
		methyl-*tert*-butylether
	anti-oxidants	*ortho*-alkylated phenols
		p-phenylenediamine
		aminophenols
		2,6-di-*tert*-butyl-p-cresol
	metal activators	N,N-disalicylidene-1,2-diaminopropane
	lead scavengers	ethylene dibromide
		ethylene dichloride
	anti-rust agents	fatty acid amines
		sulfonates
	anti-icing agents	alcohols
		glycols
		amides
		amines
		organophosphate salts
	upper-cylinder lubricants	cycloalkane distillates
	detergents	aminohydroxy amide
	dyes	alkyl derivatives of azobenzene-4-azo-2-naphthol
		benzene-azo-2-naphthol
		p-diethylaminoazobenzene
		1,4-di-isopropylaminoanthraquinone
Diesel	ignition improvers	alkyl nitrates, alkyl nitrites
		nitro-, nitroso- compounds, peroxides

Table 2. continued

Petroleum Fuel Mixture	Type	Compounds
Diesel (continued)	combustion catalysts/ deposit modifiers	organometallics of Ba, Ca, Mn, Fe Mn, MnO Mg, MgO, MgO_2 Al_2O_3
	anti-oxidants	N,N-dialkylphenylenediamines 2,6-dialkyphenols, 2,4,6-trialkylphenols
	cold flow improvers	ethylene vinyl acetate copolymers ethylene vinyl chloride copolymers polyolefins chlorinated hydrocarbons
	metal deactivators	N,N-disalicylidene-alkyldiamines
	detergents/ dispersants	alcohols amines alkylphenols carboxylic acids sulfonates succinamides
JP-4 Fuel	anti-oxidants	alkylphenols N,N-di-*sec*-butyl-*p*-phenylenediamine
	metal deactivators	N,N-disalicylidene-1,2-propanediamine N,N-disalicylidene-1,2-cyclohexanediamine N,N-disalicylidene-1,2-ethanediamine
	icing inhibitors	carboxylates alcohols dimethylformamide ammonium dinonylnaphthalene

3.2 PETROLEUM FUEL MIXTURE SPECIFICATIONS

Table 3 contains general characteristics for petroleum fuel mixtures. For each petroleum fuel mixture, the table displays an average density (g/mL), the approximate carbon number range of the predominate *n*-alkanes, distillate characteristics, hydrocarbon compound structural classes, and typical end uses.[4, 5, 6, 7] Low end distillates are those fractions collected from distillations conducted at approximately 40°C through 200°C, middle end distillates are collected from distillations conducted at approximately 200°C through 300°C, and heavy end distillates are collected from distillations conducted at approximately 300°C to 600°C. Residual oils are comprised of high molecular weight constituents that remain following distillation and collection of the lower molecular weight distillation fractions.

3.3 IMPACT OF WEATHERING ON PETROLEUM PRODUCT COMPOSITION

When petroleum products are released into the environment, changes in product composition take place. Collectively, these changes are referred to as weathering. The main weathering processes are dissolution in water, volatilization and biodegradation. In the case of spills on land or water surfaces, photodegradation can also be significant.

Each of the weathering processes affects hydrocarbon families differently. For example, aromatics tend to be more water soluble than aliphatics, whereas aliphatics tend to be more volatile. Thus when a fuel mixture is released into the environment, the principal water contaminants are likely to be aromatics while aliphatics will be the principal air contaminants. Solubility and volatility of all compounds generally decrease with an increase in molecular weight. These topics are discussed in more detail elsewhere.[8] In general, the more water soluble and volatile compounds are lost most rapidly from contaminated soil. These compounds have the lowest molecular weight, thus there is a general shift to higher molecular weight compounds in residual materials.

The rates of weathering by dissolution in water or volatilization of individual petroleum compounds are retarded by the fact that the fuels are mixtures. For example, the solubility of pure benzene in water is approximately 1800 mg/L. The equilibrium concentration of benzene in water in contact with gasoline containing 1% benzene will be approximately 20 mg/L.[9] The solubility and volatility of individual compounds in petroleum hydrocarbon mixtures are proportional to the solubility or volatility of the compound in its pure state and its concentration in the mixture. Solubility and volatility of a compound decrease when the compound is present in a mixture.

The effects of leaching and depletion of benzene, toluene, ethylbenzene and xylenes (BTEX) from gasoline in soil have been evaluated in laboratory studies.[9] Benzene is the most soluble member of this homologous series whereas ethylbenzene and xylenes are the least soluble. Benzene was depleted relatively rapidly from the gasoline-saturated soil, while ethylbenzene and xylenes tended to increase in concentration. Leaching rates of the compounds were directly proportional to their pure-state water solubilities. Benzene is ten times more soluble than ethylbenzene or xylenes, thus it was leached ten times faster. Similar trends of increased leaching with increased water solubility would be observed for BTEX in other products and for other homologous series.

If volatilization rather than dissolution were the dominant weathering process, lower molecular homologs within each series would be depleted first. The greater a compound's volatility, the more rapid its loss from a hydrocarbon mixture. As indicated above, al-

kanes tend to be much more volatile than aromatics, thus alkanes would be lost preferentially. The trend in volatility by compound class is: alkenes = alkanes > aromatics = cycloalkanes.

Considering volatilization and dissolution trends together, one can predict the composition of fuel mixtures after release in the environment.[10] Where volatilization is the dominant process, the loss of lower molecular weight alkanes will be the most significant change in the product. In situations where dissolution is the dominant weathering process (i.e. there is contact with water and limited potential for volatilization because soil pore spaces are filled with water), the aromatics will be depleted with benzene removed most rapidly.

A third process that is almost always operative when petroleum mixtures are released in the environment is biodegradation. It has been widely demonstrated that nearly all soils and sediments have populations of bacteria and other organisms that are capable of degrading petroleum hydrocarbons. Degradation occurs both in the presence and absence of oxygen. Two key factors that determine degradation rates are oxygen supply and molecular structure. In general, degradation is more rapid under aerobic conditions. Trends in degradation rates according to structure are[11]: (1) *n*-alkanes, especially in the C_{10} to C_{25} range are degraded readily, (2) isoalkanes are degraded more slowly, (3) alkenes degrade more slowly than alkanes, (4) BTEXs are metabolized when present in concentrations which are not toxic to the microorganisms, (5) PAHs degrade more slowly than monoaromatics, and (6) degradation of higher molecular weight cycloalkanes may be very slow. These trends typically result in the depletion of the more readily degradable compounds and the accumulation of the most resistant in residues.

It has been shown that biodegradation strongly affects the composition of diesel fuel after a spill in soil.[9] At the initial stages of degradation, the *n*-alkanes are degraded selectively. Over time (weeks or months), they are completely biodegraded. The compounds most easily recognizable in the remaining diesel fuel mixture at this point are the isoprenoids, which include pristane (C_{19}) and phytane (C_{20}). These compounds are alkanes with highly branched structures. This branched structure greatly reduces the rate at which biodegradation occurs. Eventually these compounds are also degraded, leaving behind a complex residue. The limited composition data available for these complex mixtures indicate that there are no detectable BTEXs and the concentrations of carcinogenic PAHs are very low.[9]

Weathered petroleum mixtures are complex and often do not contain significant quantities of individual carcinogenic compounds that alone are the limiting factors in site cleanups. The approach which has often been taken in the risk assessment of weathered mixtures has been based on "Total Petroleum Hydrocarbons" *(TPH)* measurements. TPH measurements are widely used in part because they are relatively straightforward and inexpensive. However, there are some inherent problems with using TPH measurements in risk analysis. These limitations motivated a coalition of individuals representing industry, government and academia to found the Total Petroleum Hydrocarbon Criteria Working Group. The Working Group efforts provide an improved approach for evaluating noncancer risk at petroleum contaminated sites. The approach establishes a way for complex petroleum mixtures to be evaluated as a combination of fractions where each fraction is treated like an individual chemical with appropriate toxicity criteria.

Table 3. General Characteristics of Individual Petroleum Fuel Mixtures

Petroleum Fuel Mixture	Density	Alkane Carbon Number Range	Distillate Characteristics
Gasoline	~0.73g/mL	n-C4 through n-C12	low-end distillate boiling point range of 40-200°C
Kerosene	~0.80g/mL	n-C6 through n-C16	middle distillate boiling point range of 150-300°C
JP-4 fuel	~0.75g/mL	n-C5 through n-C14	middle distillate mixture of gasoline (65%) and petroleum distillates (35%) boiling point range of 150-275°C
JP-5 fuel	~0.82g/mL	n-C8 throug n-C17	middle distillate specially blended kerosene boiling point range of 150-275°C
JP-7 fuel		n-C10 through n-C17	middle distillate high flash point kerosene boiling point range of 150-275°C
JP-8 fuel	~0.81g/mL	n-C7 through n-C18	middle distillate kerosene modeled on Jet A-1 boiling point range of 150-275°C

Compound Classes	End Use
high concentrations of BTEXs*, monoaromatics and branched alkanes lower concentrations of n-alkanes, alkenes, cycloalkanes, and naphthalenes. very low concentrations of PAHs.	automotive spark-ignition engine
high concentrations of cycloalkanes and n-alkanes. lower concentrations of monoaromatics and branched alkanes. very low concentrations of BTEXs and PAHs.	critical kerosene burners
high concentrations of n-alkanes and cycloalkanes. lower concentrations of n-alkanes, BTEXs and monoaromatics. very low concentrations of PAHs.	aviation turbine engines
high concentrations of cycloalkanes and n-alkanes. lower concentrations of monoaromatics and branched alkanes. very low concentrations of BTEXs and PAHs.	aviation turbine engines shipboard engines
high concentrations of cycloalkanes and n-alkanes. lower concentrations of monoaromatics and branched alkanes. very low concentrations of BTEXs and PAHs.	aviation turbine engines
high concentrations of cycloalkanes and n-alkanes. lower concentrations of monoaromatics and branched alkanes. very low concentrations of BTEXs and PAHs	aviation turbine engines

Table 3. continued

Petroleum Fuel Mixture	Density	Alkane Carbon Number Range	Distillate Characteristics
Diesel (#2)	~0.83g/mL	n-C8 through n-C21	middle distillate boiling point range of 200-325^{o}C
No.2 fuel oil	~0.90g/mL	n-C8 through n-C21	middle distillate boiling point range of 200-325^{o}C
No.6 fuel oil	~0.95g/mL	n-C12 through beyond n-C34	residual oil boiling point range of 350-700^{o}C
Lubricating and motor oils		n-C18 through beyond n-C34	heavy end distillate boiling point range of 325-600^{o}C
Crude oil	~0.94g/mL	n-C1 through beyond n-C34	feedstock

* BTEXs = benzene, toluene, xylenes and ethylbenzene

Compound Classes	End Use
high concentrations of n-alkanes lower concentrations of branched alkanes, cycloalkanes, monoaromatics, naphthalenes, and PAHs. very low concentrations of BTEXs.	high-speed engines
high concentrations of n-alkanes lower concentrations of branched alkanes, cycloalkanes, monoaromatics, naphthalenes, and PAHs. very low concentrations of BTEXs.	domestic burners medium capacity commercial industrial burners
high concentrations of n-alkanes and cycloalkanes. lower concentrations of naphthalenes and PAHs. very low concentrations of BTEXs.	commercial burners industrial burners
lower concentrations of barium. high concentrations of branched alkanes and cycloalkanes. very low concentrations of BTEXs and PAHs.	internal combustion engines
high concentrations of n-alkanes, branched alkanes and cycloalkanes. lower concentrations of BTEXs, PAHs and naphthalenes. variable concentrations of sulfur heterocyclics.	

4.1 DATA SOURCES DISCUSSION

The composition data in this document were obtained through efforts of the Total Petroleum Hydrocarbon Criteria Working Group. The Working Group searched the published technical literature and contacted government and private sector laboratories involved in petroleum hydrocarbon mixture analysis. Individuals were contacted at the U.S. Environmental Protection Agency, U.S. Air Force, U.S. Navy, U.S. Department of Energy and the oil industry research centers. The search for data was conducted over a period of nearly one year. It was comprehensive in both scale and scope.

The principal sources of data reported in this volume are journal articles and book chapters identified in two bibliographic compilations. One compilation was obtained from the American Petroleum Institute.[12] The second was created by manually searching fifteen peer-reviewed analytical, environmental and petroleum chemistry journals published between 1984 and 1995. In addition, manuscripts published in the book series *Hydrocarbon Contaminated Soils* published between 1987 and 1994 were similarly searched. The manual approach was taken in these searches since electronic keyword searches yielded few useful citations.[9] For example, keyword searches of the *Chemical Abstracts* provided thousands of citations. However, when keywords such as "composition" were added, less than ten citations remained. In addition, the data contained in the cited articles were in most cases not compound-specific. Instead, they were reported according to group type, such as aromatics or aliphatics. Manual searching, although tedious, allowed identification of data in documents which primarily addressed topics other than product composition but which contained compound-specific data (e.g. studies on the emissions of hydrocarbons from gasoline and diesel engines).

Copies of all cited articles were obtained, petroleum fuel mixture composition data were compiled, and the data were entered into a Microsoft Access® database. Selected data contributed from oil and government laboratories were also included.

Each of the data-sets was carefully checked by an expert panel of petroleum and environmental chemists. Citations were checked to determine whether they were from a primary or secondary source. Secondary source refers to data that were not produced by the authors of a study but were included by citation from another source. Wherever possible, all data were traced to their original source. For No.6 fuel oil, one or two sets of data were found to be reported by many different authors. Elimination of repeated citations greatly reduced the number of citations and provided a more accurate picture of the average values reported. The data review also involved checking for uniformity of nomenclature, reporting units, and applying a "test of reasonableness". This "test" was simply a determination by experienced petroleum analytical chemists of whether the data were within an expected range for a given product type.

4.2 DATA GAPS AND RESEARCH NEEDS

While providing useful insights into the composition of petroleum fuel mixtures and supporting preliminary risk-based evaluations of sites, the available data are not ideal for use in detailed risk-based analysis. They are compiled from a variety of sources

over a ten to fifteen year period, with studies occurring for different reasons at different laboratories. Ideally these data would be generated as part of a systematic effort to characterize the composition of the mixtures.

More significantly, very few data were identified that characterized the composition of weathered petroleum fuel mixtures. There are major qualitative and quantitative differences between fresh and weathered petroleum fuel mixtures. As discussed in Section 3.3, the trend is toward depletion of the more water soluble, more volatile and more easily biodegradable compounds. Thus, the constituents of the weathered mixture are generally less mobile in the environment. Consequently, the overall environmental hazard posed by weathered petroleum mixtures may be less than that posed by fresh mixtures. The extent to which this reduced hazard occurs with weathering or whether toxic substances are concentrated in weathered mixtures has not been documented.

5.0 PETROLEUM FUEL MIXTURE COMPOSITION DATA

5.1 INTRODUCTION TO PETROLEUM FUEL MIXTURE COMPOSITION DATA TABLES

The petroleum fuel mixture composition data is presented in two sets of tables. The first set of data tables (Tables 4-14) reports summary statistics of petroleum constituent weight percent data for petroleum mixtures. The second set of tables (Appendix I) reports petroleum constituent weight percent data and data quality information for individual samples included in the database. Appendix I is not presented in entirety in this publication but may be obtained electronically at www.aehs.com.

The data in Tables 4-14 are summations of data from the second set of tables (Appendix I) organized by petroleum fuel mixture specification. The total number of data points listed in the first set of tables is a summation of the number of data point entries for all samples within the petroleum fuel mixture specification. Summary statistics should include weight percent values for all data points, but individual weight percent values were not always reported in the original literature sources. For example, some studies only report an average weight percent value for twenty measurements rather than the twenty individual weight percent values. The summary statistic calculations for average weight percent, standard deviation and coefficient of variation were all weighted to include the total number of data points.

To account for missing individual weight percent values, average weight percent values were calculated according to Equation 1. Minimum and maximum values for weight percents are listed when more than one data point was available.

$$\text{average weight percent} = \frac{\sum (W \times D)}{\sum D} \quad (1)$$

where:

W = weight percent

D = number of data points

When more than two entries were made, the standard deviation of the weight percents was calculated according to Equation 2.

$$\text{standard deviation} = \sqrt{\left(\sum(W \times W) - \frac{(\sum W) \times (\sum W)}{\sum D}\right) \times \left(\frac{1}{\sum D - 1}\right)} \quad (2)$$

where:

W = weight percent

D = number of data points

When a standard deviation value was calculated and reported, the coefficient of variation was also reported with the value being calculated according to Equation 3.

$$\text{coefficient of variation} = \frac{S}{A} \times 100 \quad (3)$$

where:

S = standard deviation

A = average weight percent

The average weight percent, minimum, maximum, standard deviation, and coefficient of variation values are all reported to two significant figures in scientific notation format.

The tables included in Appendix I list individual sample data as reported in the specified literature sources. Each table lists a “sample #” which is the name of the sample as specified in the source literature, and that name is preceded by a number which identifies the literature source as listed in Section 6.2. Each table also lists the petroleum fuel mixture, the literature source, the compounds that were detected, and the weight percent contribution of each compound. Compounds are further described by carbon number and general compound class. Weight percent data are presented to two significant figures in scientific notation format. In most cases, the weight percent value is representative of a single data point. There are cases where the weight percent value is representative of more than one data point. The number of data points that contributed to the reported weight percent value is listed in the table.

5.2 SUMMARY OF COMPOSITION DATA

Table 4. Summary of Composition Data for Gasoline Fuel Oil

compound class	carbon #	compound
Alkenes		Total Alkenes
	4	1,3-Butadiene
	4	cis-2-Butene
	4	trans-2-Butene
	5	2-Methyl-1-butene
	5	2-Methyl-2-butene
	5	cis-2-Pentene
	5	trans-2-Pentene
Alkyl-Monoaromatics	6	Benzene
	7	Toluene
	8	Ethylbenzene
	8	m-Xylene
	8	o-Xylene
	8	p-Xylene
	9	1,2,4-Trimethylbenzene
	9	1,3,5-Trimethylbenzene
	9	1-Methyl-2-ethylbenzene
	9	1-Methyl-3-ethylbenzene
	9	1-Methyl-4-ethylbenzene
Branched Alkanes	4	Isobutane
	5	Isopentane
	6	2,2-Dimethylbutane
	6	2,3-Dimethylbutane
	6	2-Methylpentane
	6	3-Methylpentane
	7	2,4-Dimethylpentane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.0E+01	8.4E+00	1.2E+01	2.2E+00	2.2E+01	124
3.7E-03	1.0E-03	6.0E-03	8.9E-04	2.4E+01	124
3.1E-01	2.0E-01	4.5E-01	6.8E-02	2.2E+01	124
3.6E-01	2.3E-01	5.3E-01	7.9E-02	2.3E+01	124
5.4E-01	4.8E-01	6.2E-01	1.1E-01	2.1E+01	124
1.1E+00	9.7E-01	1.2E+00	2.2E-01	2.1E+01	124
3.9E-01	3.5E-01	4.4E-01	8.0E-02	2.1E+01	124
7.2E-01	6.5E-01	8.0E-01	1.5E-01	2.1E+01	124
1.9E+00	1.6E+00	2.3E+00	4.1E-01	2.2E+01	124
8.1E+00	6.4E+00	1.0E+01	1.8E+00	2.2E+01	124
1.7E+00	1.4E+00	2.0E+00	3.7E-01	2.2E+01	124
4.6E+00	3.9E+00	5.4E+00	1.0E+00	2.2E+01	124
2.5E+00	2.1E+00	3.1E+00	5.6E-01	2.2E+01	124
1.9E+00	1.6E+00	2.3E+00	4.1E-01	2.2E+01	124
3.0E+00	2.5E+00	3.3E+00	6.5E-01	2.2E+01	124
9.8E-01	8.4E-01	1.1E+00	2.1E-01	2.2E+01	124
7.1E-01	6.2E-01	7.8E-01	1.6E-01	2.2E+01	124
1.8E+00	1.5E+00	2.0E+00	4.0E-01	2.2E+01	124
8.0E-01	6.6E-01	9.1E-01	1.8E-01	2.2E+01	124
1.7E+00	8.0E-01	2.6E+00	4.1E-01	2.4E+01	124
7.9E+00	7.1E+00	8.8E+00	1.7E+00	2.2E+01	124
4.9E-01	4.0E-01	6.4E-01	1.1E-01	2.2E+01	124
1.0E+00	9.7E-01	1.1E+00	2.2E-01	2.1E+01	124
3.9E+00	3.2E+00	4.5E+00	8.4E-01	2.2E+01	124
2.5E+00	2.1E+00	2.9E+00	5.4E-01	2.2E+01	124
8.3E-01	5.6E-01	1.2E+00	1.9E-01	2.3E+01	124

Table 4. continued

compound class	carbon #	compound
Branched Alkanes (continued)	7	2-Methylhexane
	7	3-Methylhexane
	8	2,2,4-Trimethylpentane
	8	2,3,3-Trimethylpentane
	8	2,3,4-Trimethylpentane
	8	2,3-Dimethylhexane
	8	2,4-Dimethylhexane
	8	3-Methylheptane
Cycloalkanes	5	Cyclopentane
	6	Cyclohexane
	6	Methylcyclopentane
	7	Methylcyclohexane
n-Alkanes	4	n-Butane
	5	n-Pentane
	6	n-Hexane
	7	n-Heptane
Naphthalenes		Total Naphthalenes
	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
Oxygenates	5	Methyl-tert-butylether
Total Aromatics		Total Aromatics
Total Monoaromatics		Total Benzene, Toluene and Xylenes
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
3.0E+00	2.5E+00	3.8E+00	6.5E-01	2.2E+01	124
1.7E+00	1.6E+00	1.9E+00	3.7E-01	2.1E+01	124
2.4E+00	8.7E-01	4.2E+00	5.9E-01	2.5E+01	124
6.6E-01	2.0E-01	1.3E+00	1.7E-01	2.6E+01	124
9.7E-01	3.5E-01	1.8E+00	2.4E-01	2.5E+01	124
3.9E-01	2.5E-01	5.8E-01	8.9E-02	2.3E+01	124
4.4E-01	3.1E-01	6.1E-01	9.7E-02	2.2E+01	124
7.5E-01	6.2E-01	8.7E-01	1.6E-01	2.2E+01	124
4.7E-01	3.4E-01	6.1E-01	1.1E-01	2.2E+01	124
3.9E-01	2.3E-01	6.0E-01	9.3E-02	2.3E+01	124
1.8E+00	1.4E+00	2.3E+00	4.0E-01	2.2E+01	124
5.8E-01	3.9E-01	7.5E-01	1.3E-01	2.2E+01	124
4.7E+00	2.6E+00	6.5E+00	1.1E+00	2.3E+01	124
3.9E+00	3.0E+00	4.9E+00	8.6E-01	2.2E+01	124
2.4E+00	1.8E+00	3.2E+00	5.3E-01	2.2E+01	124
1.1E+00	1.0E+00	1.2E+00	2.4E-01	2.1E+01	124
5.8E+00	4.1E+00	7.2E+00	1.3E+00	2.2E+01	124
2.5E-01	1.5E-01	3.6E-01	5.7E-02	2.2E+01	124
7.0E-02	4.0E-02	1.1E-01	1.6E-02	2.3E+01	124
1.8E-01	1.0E-01	2.9E-01	4.3E-02	2.3E+01	124
3.3E-01	1.0E-02	7.9E-01	1.0E-01	2.7E+01	124
3.5E+01	2.9E+01	3.8E+01	7.5E+00	2.2E+01	124
1.9E+01	1.6E+01	2.4E+01	4.2E+00	2.2E+01	124
4.7E+01	4.5E+01	5.0E+01	1.0E+01	2.1E+01	124

Table 5. Summary of Composition Data for Kerosene Fuel Oil

compound class	carbon #	compound
Alkyl-Monoaromatics	10	1,2,3,4-Tetramethylbenzene
Branched Alkanes	10	Isodecane
	11	Isoundecane
	12	Isododecane
	13	Isotridecane
	14	Isotetradecane
Diaromatics (Except Naphthalenes)	13	Fluorene
Monoaromatics	9	Indene
	10	Tetralin
	11	1-Methyltetralin
	11	2-Methyltetralin
n-Alkanes	7	n-Heptane
	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
	18	n-Octadecane
	19	n-Nonadecane
	20	n-Eicosane
	21	n-Heneicosane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.1E+00					1
1.3E+00					1
1.2E+00					1
1.2E+00					1
9.0E-01					1
6.0E-01					1
4.2E-03					1
2.6E-04					1
2.7E-01					1
6.5E-01					1
6.8E-01					1
7.3E-01	1.0E-01	1.4E+00			2
1.6E+00	3.0E-01	3.1E+00	1.4E+00	8.6E+01	3
2.3E+00	4.8E-01	5.6E+00	2.9E+00	1.3E+02	3
3.2E+00	1.7E+00	5.6E+00	2.1E+00	6.6E+01	3
5.2E+00	4.0E+00	6.1E+00	1.1E+00	2.0E+01	3
6.8E+00	2.4E+00	1.4E+01	4.8E+00	7.0E+01	4
3.3E+00	2.1E+00	5.2E+00	1.7E+00	5.2E+01	3
3.3E+00	2.0E+00	4.7E+00			2
2.2E+00	2.2E+00	2.3E+00			2
7.0E-01					1
4.0E-01					1
3.0E-01					1
2.0E-01					1
1.0E-01					1
1.0E-01					1

Table 5. continued

compound class	carbon #	compound
Naphthalenes	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	12	1,4-Dimethylnaphthalene
Polynuclear Aromatics	12	Acenaphthene
	12	Acenaphthylene
	14	Anthracene
	14	Phenanthrene
	15	2-Methylanthracene
	16	9,10-Dimethylanthracene
	16	Fluoranthene
	16	Pyrene
	17	2,3-Benzofluorene
	17	Benzo(a)fluorene
	20	7,12-Dimethylbenz(a)anthracene

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
3.1E-01	1.5E-01	4.6E-01			2
5.4E-01	2.5E-01	8.4E-01			2
1.1E+00	3.4E-01	1.8E+00			2
1.9E-01					1
4.7E-03					1
4.5E-03					1
1.2E-04					1
5.8E-02					1
4.6E-04					1
7.1E-04					1
8.6E-04					1
2.4E-04					1
1.2E-04					1
9.0E-05					1
2.0E-03					1

Table 6. Summary of Composition Data for JP-4 Fuel Oil

compound class	carbon #	compound
Alkyl-Monoaromatics	6	Benzene
	7	Toluene
	8	Ethylbenzene
	8	m-Xylene
	8	o-Xylene
	8	p-Xylene
	9	1,2,4-Trimethylbenzene
	9	1,3,5-Trimethylbenzene
	9	1-Ethyl-3-methylbenzene
	9	1-Methyl-2-ethylbenzene
	9	1-Methyl-3-ethylbenzene
	9	1-Methyl-4-ethylbenzene
	9	Isopropylbenzene
	9	n-Propylbenzene
	10	1,2,3,4-Tetramethylbenzene
	10	1,2-Dimethyl-4-ethylbenzene
	10	1,3-Diethylbenzene
	10	1,3-Dimethyl-5-ethylbenzene
	10	1,4-Dimethyl-2-ethylbenzene
	10	1-Methyl-2-isopropylbenzene
	10	1-Methyl-4-propylbenzene
Branched Alkanes	4	Isobutane
	5	2-Methylbutane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
4.7E-01	4.7E-01	5.0E-01			107
1.6E+00	1.3E+00	1.6E+00			107
6.6E-01	3.7E-01	6.9E-01			11
9.6E-01					1
1.0E+00					1
3.5E-01					1
1.0E+00					1
4.2E-01					1
5.7E-01					105
2.3E-01					1
4.9E-01					1
4.3E-01					1
3.0E-01					1
7.1E-01					1
7.5E-01					1
7.7E-01					1
4.6E-01					1
6.1E-01					1
7.0E-01					1
2.9E-01					1
4.0E-01					1
6.6E-01					1
5.9E-01					106

Table 6. continued

compound class	carbon #	compound
Branched Alkanes (continued)	6	2,2-Dimethylbutane
	6	2-Methylpentane
	6	3-Methylpentane
	7	2,2-Dimethylpentane
	7	2,3-Dimethylpentane
	7	2-Methylhexane
	7	3,3-Dimethylpentane
	7	3-Ethylpentane
	7	3-Methylhexane
	8	2,2,3,3-Tetramethylbutane
	8	2,2-Dimethylhexane
	8	2,4-Dimethylhexane
	8	2,5-Dimethylhexane
	8	2-Methylheptane
	8	3,3-Dimethylhexane
	8	3-Methylheptane
	8	4-Methylheptane
	9	2,5-Dimethylheptane
	9	2-Methyloctane
	9	3,4-Dimethylheptane
	9	3-Ethylheptane
	9	3-Methyloctane
	9	4-Ethylheptane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.3E-01	1.0E-01	1.3E-01			96
1.5E+00	1.3E+00	1.5E+00			107
1.1E+00	8.9E-01	1.1E+00			107
2.5E-01					1
6.2E-01					106
1.3E+00	1.3E+00	2.3E+00			107
9.4E-02					106
1.4E-01					106
1.5E+00	1.5E+00	2.0E+00			107
5.8E-01	2.4E-01	5.8E-01			107
7.1E-01					1
5.8E-01					1
3.7E-01					1
2.7E+00					1
2.6E-01					1
3.0E+00					1
9.2E-01					1
5.2E-01					1
8.8E-01					1
4.3E-01					1
1.1E-01					94
7.9E-01					1
1.8E-01					1

Table 6. continued

compound class	carbon #	compound
Branched Alkanes (continued)	9	4-Methyloctane
	12	2-Methylundecane
	13	2,6-Dimethylundecane
Cycloalkanes	6	Cyclohexane
	6	Methylcyclopentane
	7	cis-1,2-Dimethylcyclopentane
	7	cis-1,3-Dimethylcyclopentane
	7	Ethylcyclopentane
	7	Methylcyclohexane
	7	trans-1,2-Dimethylcyclopentane
	7	trans-1,3-Dimethylcyclopentane
	7	trans-2,3-Dimethylcyclopentane
	8	1,2,3-Trimethylcyclopentane
	8	1,2,4-Trimethylcyclopentane
	8	cis-1,3-Dimethylcyclohexane
	8	Dimethylcyclohexane
	9	1,1,3-Trimethylcyclohexane
	9	1,3,5-Trimethylcyclohexane
	9	1-Methyl-2-ethylcyclohexane
	9	1-Methyl-3-ethylcyclohexane
	9	1-Methyl-4-ethylcyclohexane
	10	n-Butylcyclohexane
n-Alkanes	4	n-Butane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
8.6E-01					1
6.4E-01					1
7.1E-01					1
1.2E+00	1.2E+00	1.2E+00			107
1.4E+00	1.2E+00	1.4E+00			107
5.4E-01					1
4.2E-01	3.4E-01	4.2E-01			107
2.6E-01	2.6E-01	2.6E-01			107
2.8E+00	2.3E+00	2.8E+00			107
7.4E-01					106
4.5E-01					106
3.6E-01					1
2.5E-01					1
2.5E-01					1
4.2E-01					1
4.3E-01					1
4.8E-01					1
9.9E-01					1
3.9E-01					1
1.7E-01					1
4.8E-01					1
7.0E-01					1
1.7E-01	1.2E-01	1.7E-01			93

Table 6. continued

compound class	carbon #	compound
n-Alkanes (continued)	5	n-Pentane
	6	n-Hexane
	7	n-Heptane
	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
Naphthalenes	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	12	2,6-Dimethylnaphthalene

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
9.2E-01	9.2E-01	1.1E+00			107
2.4E+00	2.2E+00	2.4E+00			107
2.8E+00	2.8E+00	3.7E+00			107
2.2E+00	2.2E+00	3.8E+00			107
1.9E+00	1.9E+00	2.3E+00			107
1.6E+00	1.6E+00	2.2E+00			107
1.5E+00	1.5E+00	2.3E+00			107
1.0E+00	1.0E+00	2.0E+00			105
8.3E-01	8.2E-01	1.5E+00			103
7.3E-01					1
1.9E-01					95
7.3E-02					76
2.5E-01	2.5E-01	5.0E-01			91
4.1E-02	3.3E-02	7.8E-01			93
1.4E-01	1.4E-01	5.6E-01			101
2.5E-01					1

Table 7. Summary of Composition Data for JP-5 Fuel Oil

compound class	carbon #	compound
Alkenes	13	Tridecene
Alkyl-Monoaromatics	8	m-Xylene
	8	o-Xylene
	9	1,2,4-Trimethylbenzene
	10	1,2,3,4-Tetramethylbenzene
	10	1,3-Diethylbenzene
	10	1,4-Diethylbenzene
	12	1,2,4-Triethylbenzene
	13	1-tert-Butyl-3,4,5-trimethylbenzene
	13	n-Heptylbenzene
	14	n-Octylbenzene
	15	1-Ethylpropylbenzene
Branched Alkanes	9	3-Methyloctane
	10	2,4,6-Trimethylheptane
	11	2-Methyldecane
	11	4-Methyldecane
	12	2,6-Dimethyldecane
	12	2-Methylundecane
	13	2,6-Dimethylundecane
Cycloalkanes	9	1,1,3-Trimethylcyclohexane
	9	1,3,5-Trimethylcyclohexane
	10	n-Butylcyclohexane
	12	Phenylcyclohexane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
4.5E-01					1
1.3E-01					1
9.0E-02					1
3.7E-01					1
1.5E+00					1
6.1E-01					1
7.7E-01					1
7.2E-01					1
2.4E-01					1
2.7E-01					1
7.8E-01					1
1.2E+00					1
7.0E-02					1
7.0E-02					1
6.1E-01					1
7.8E-01					1
7.2E-01					1
1.4E+00					1
2.0E+00					1
5.0E-02					1
9.0E-02					1
9.0E-01					1
8.2E-01					1

Table 7. continued

compound class	carbon #	compound
Cycloalkanes (continued)	13	Heptylcyclohexane
Diaromatics (Except Naphthalenes)	12	Biphenyl
n-Alkanes	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
Naphthalenes	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	12	1-Ethylnaphthalene
	12	2,3-Dimethylnaphthalene
	12	2,6-Dimethylnaphthalene

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
9.9E-01					1
7.0E-01					1
1.2E-01					1
3.8E-01					1
1.8E+00					1
4.0E+00					1
3.9E+00					1
3.5E+00					1
2.7E+00					1
1.7E+00					1
1.1E+00					1
1.2E-01					1
5.7E-01					1
1.4E+00					1
1.4E+00					1
3.2E-01					1
4.6E-01					1
1.1E+00					1

Table 8. Summary of Composition Data for JP-7 Fuel Oil

compound class	carbon #	compound
Alkyl-Monoaromatics		Total Alkyl-Monoaromatics
	8	1,2-Diethylbenzene
	10	1,2-Dimethyl-3-ethylbenzene
	10	1,2-Dimethyl-4-ethylbenzene
	10	1,3-Dimethyl-2-ethylbenzene
	10	1,3-Dimethyl-4-ethylbenzene
	10	1,4-Diethylbenzene
	10	1,4-Dimethyl-2-ethylbenzene
	10	1-Methyl-2-isopropylbenzene
	10	1-Methyl-2-propylbenzene
	10	1-Methyl-3-propylbenzene
	10	1-Methyl-4-isopropylbenzene
	10	1-Methyl-4-propylbenzene
	10	n-Butylbenzene
	11	2-Methylbutylbenzene
	11	Pentylbenzene
	12	1,2,4-Triethylbenzene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.6E+00					1
1.8E-01					1
2.1E-01					1
1.0E-01					1
5.9E-02					1
2.0E-02					1
2.0E-02					1
1.8E-01					1
5.9E-02					1
4.0E-02					1
5.9E-02					1
9.9E-03					1
3.0E-02					1
9.9E-03					1
6.9E-02					1
1.9E-01					1
4.0E-02					1

Table 8. continued

compound class	carbon #	compound
Alkyl-Monoaromatics (continued)	12	1-tert-Butyl-3,5-dimethylbenzene
Cycloalkanes	10	n-Butylcyclohexane
n-Alkanes	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
Naphthalenes	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
Total Cycloalkanes		Total Cycloalkanes
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
6.9E-02					1
8.3E-02					1
2.5E-01					1
7.7E+00					1
1.2E+01					1
5.0E+00					1
2.3E+00					1
7.7E-01					1
2.0E-01					1
4.2E-02					1
7.2E-01					1
4.4E-02					1
1.0E-01					1
3.5E-01					1
8.1E+01					1

Table 9. Summary of Composition Data for JP-8 Fuel Oil

compound class	carbon #	compound
Alkenes	13	Tridecene
Alkyl-Monoaromatics	8	m-Xylene
	8	o-Xylene
	9	1,2,3-Trimethylbenzene
	10	1,2,3,4-Tetramethylbenzene
	10	1,3-Dimethyl-5-ethylbenzene
	10	1-Methyl-2-isopropylbenzene
	12	1,2,4-Triethylbenzene
	12	1,3,5-Triethylbenzene
	13	n-Heptylbenzene
	14	n-Octylbenzene
	15	1-Ethylpropylbenzene
Branched Alkanes	9	3-Methyloctane
	10	2,4,6-Trimethylheptane
	11	2-Methyldecane
	12	2,6-Dimethyldecane
	12	2-Methylundecane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
7.3E-01					1
6.0E-02					1
6.0E-02					1
2.7E-01					1
1.1E+00					1
6.2E-01					1
5.6E-01					1
9.9E-01					1
6.0E-01					1
2.5E-01					1
6.1E-01					1
9.9E-01					1
4.0E-02					1
7.0E-02					1
4.1E-01					1
6.6E-01					1
1.2E+00					1

Table 9. continued

compound class	carbon #	compound
Branched Alkanes (continued)	13	2,6-Dimethylundecane
Cycloalkanes	9	1,1,3-Trimethylcyclohexane
	9	1,3,5-Trimethylcyclohexane
	9	1-Methyl-4-ethylcyclohexane
	9	Propylcyclohexane
	10	n-Butylcyclohexane
	12	Hexylcyclohexane
	12	Phenylcyclohexane
	13	Heptylcyclohexane
Diaromatics (Except Naphthalenes)	12	Biphenyl
n-Alkanes	7	n-Heptane
	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
2.1E+00					1
6.0E-02					1
6.0E-02					1
1.0E-01					1
1.4E-01					1
7.4E-01					1
9.3E-01					1
8.7E-01					1
1.0E+00					1
6.3E-01					1
3.0E-02					1
9.0E-02					1
3.1E-01					1
1.3E+00					1
4.1E+00					1
4.7E+00					1
4.4E+00					1

Table 9. continued

compound class	carbon #	compound
n-Alkanes (continued)	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
	18	n-Octadecane
Naphthalenes	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	12	1-Ethylnaphthalene
	12	2,3-Dimethylnaphthalene
	12	2,6-Dimethylnaphthalene

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
3.0E+00					1
1.6E+00					1
4.5E-01					1
8.0E-02					1
2.0E-02					1
1.1E+00					1
1.8E+00					1
1.5E+00					1
3.3E-01					1
3.6E-01					1
1.3E+00					1

Table 10. Summary of Composition Data for Diesel (#2) Fuel Oil

compound class	carbon #	compound
Alkenes		Total Alkenes
Alkyl-Monoaromatics		Total Alkyl-Monoaromatics
	6	Benzene
	7	Toluene
	8	Ethylbenzene
	8	m+p-Xylenes
	8	o-Xylene
	8	Total Xylenes
	9	1,3,5-Trimethylbenzene
	9	n-Propylbenzene
	10	1-Methyl-4-isopropylbenzene
	10	n-Butylbenzene
Branched Alkanes	12	3-Methylundecane
	13	2-Methyldodecane
	14	3-Methyltridecane
	15	2-Methyltetradecane
	19	Pristane
	20	Phytane
Cycloalkanes		Total Dicycloalkanes
		Tota Monocycloalkanes
		Total Tetracycloalkanes
		Total Tricycloalkanes
Diaromatics (Except Naphthalenes)		Total Fluorenes
	12	Biphenyl

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.3E+00	2.0E-01	2.2E+00	6.8E-01	5.4E+01	8
6.2E+00	1.8E+00	8.1E+00	2.1E+00	3.4E+01	20
2.9E-02	2.6E-03	1.0E-01	4.7E-02	1.6E+02	4
1.8E-01	6.9E-03	7.0E-01	2.7E-01	1.5E+02	6
6.8E-02	7.0E-03	2.0E-01	7.2E-02	1.1E+02	6
2.2E-01	1.8E-02	5.1E-01	1.8E-01	8.3E+01	5
4.3E-02	1.2E-03	8.5E-02	3.8E-02	8.9E+01	5
5.0E-01					1
1.8E-01	9.0E-02	2.4E-01	7.8E-02	4.4E+01	3
3.9E-02	3.0E-02	4.8E-02	9.0E-03	2.3E+01	3
1.5E-02	3.0E-03	2.6E-02			2
3.8E-02	3.1E-02	4.6E-02			2
1.7E-01	9.0E-02	2.8E-01	6.3E-02	3.6E+01	6
2.8E-01	1.5E-01	5.2E-01	1.1E-01	4.1E+01	7
1.9E-01	1.3E-01	3.0E-01	5.8E-02	3.0E+01	7
4.8E-01	3.4E-01	6.3E-01	1.1E-01	2.3E+01	7
6.0E-01	3.5E-01	8.1E-01	1.6E-01	2.6E+01	7
5.0E-01	3.5E-01	5.9E-01	8.9E-02	1.8E+01	7
1.4E+01	3.7E+00	1.8E+01	3.2E+00	2.3E+01	21
1.9E+01	1.3E+01	3.1E+01	4.0E+00	2.1E+01	20
1.0E-01					1
6.2E+00	1.6E+00	1.3E+01	2.6E+00	4.2E+01	21
5.6E-01	3.0E-02	1.4E+00	7.3E-01	1.3E+02	3
6.3E-02	6.2E-03	1.2E-01			2

Table 10. continued

compound class	carbon #	compound
Diaromatics (Except Naphthalenes) (continued)	13	Fluorene
	13	Total Methylbiphenyls
	14	Total Methylfluorenes
	15	Total Dimethylfluorenes
Inorganics		Total Nitrogen
		Total Sulfur
		Water
Metals		Arsenic
		Cadmium
		Chromium
		Iron
		Manganese
		Molybdenum
		Zinc
Monoaromatics		Total Benzocycloparaffins
		Total Benzodicycloparaffins
		Total Dinaphthenobenzenes
		Total Indenes
	10	Total Indans and Tetralins
n-Alkanes	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
8.6E-02	3.4E-02	1.5E-01	4.3E-02	5.0E+01	13
5.3E-02					1
2.0E-01	9.0E-02	3.8E-01	1.1E-01	5.4E+01	6
4.2E-01					1
9.1E-03	7.0E-05	5.6E-02	1.2E-02	1.3E+02	20
7.2E-02	4.1E-03	4.9E-01	1.4E-01	1.9E+02	27
5.2E-04	1.5E-04	7.3E-04	2.3E-04	4.4E+01	8
7.1E-06					6
4.9E-05					6
1.7E-04					6
3.7E-03					6
3.2E-04					6
1.4E-05					6
3.1E-04					6
6.3E+00	6.0E+00	6.6E+00			2
3.0E+00	3.0E+00	3.0E+00			2
1.8E+00					1
3.1E+00	7.0E-01	5.6E+00	1.5E+00	4.8E+01	17
5.9E+00	1.2E+00	1.0E+01	2.6E+00	4.4E+01	18
1.1E-01	1.0E-01	1.3E-01			2
3.8E-01	1.9E-01	4.9E-01	1.1E-01	3.0E+01	9
7.8E-01	2.8E-01	1.2E+00	3.3E-01	4.2E+01	7
1.4E+00	5.7E-01	2.3E+00	5.5E-01	4.0E+01	7
1.7E+00	1.0E+00	2.5E+00	5.2E-01	3.1E+01	7

Table 10. continued

compound class	carbon #	compound
n-Alkanes (continued)	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
	18	n-Octadecane
	19	n-Nonadecane
	20	n-Eicosane
	21	n-Heneicosane
	22	n-Docosane
	24	n-Tetracosane
Naphthalenes		Total Naphthalenes
	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	11	Total Methylnaphthalenes
	12	1,3-Dimethylnaphthalene
	12	1,4-Dimethylnaphthalene
	12	1,5-Dimethylnaphthalene
	12	Total Dimethylnaphthalenes
	13	Total Trimethylnaphthalenes
Other		2-Azapyrene
		Total Thioaromatics
	10	Ethylhexyl nitrate

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
2.1E+00	1.5E+00	2.8E+00	4.3E-01	2.1E+01	7
1.9E+00	6.1E-01	2.7E+00	6.6E-01	3.4E+01	9
2.6E+00	1.9E+00	3.1E+00	3.9E-01	1.5E+01	7
2.3E+00	1.5E+00	2.8E+00	4.6E-01	2.0E+01	7
2.2E+00	1.4E+00	2.9E+00	4.6E-01	2.1E+01	7
1.6E+00	1.2E+00	2.0E+00	3.1E-01	2.0E+01	7
1.0E+00	7.3E-01	1.5E+00	2.6E-01	2.5E+01	7
6.2E-01	3.7E-01	1.0E+00	2.3E-01	3.8E+01	7
4.4E-01	1.6E-01	8.3E-01	2.6E-01	5.9E+01	7
3.1E-01	1.4E-01	4.4E-01	1.3E-01	4.2E+01	4
3.5E-01					1
3.1E+00	4.1E-01	1.0E+01	2.7E+00	8.8E+01	22
2.6E-01	1.0E-02	8.0E-01	1.8E-01	7.0E+01	29
4.8E-01	7.0E-04	8.1E-01	2.6E-01	5.5E+01	8
8.9E-01	1.1E-03	1.5E+00	4.6E-01	5.2E+01	8
2.9E-01	1.4E-01	4.6E-01	1.4E-01	4.9E+01	5
9.7E-01	5.5E-01	1.3E+00	2.5E-01	2.6E+01	7
1.8E-01	1.1E-01	2.3E-01	4.2E-02	2.3E+01	7
2.9E-01	1.6E-01	3.6E-01	6.9E-02	2.4E+01	7
6.9E-01	4.9E-01	9.4E-01	2.1E-01	3.0E+01	5
2.4E-01	2.1E-02	4.0E-01	1.2E-01	5.1E+01	6
1.4E-04	1.0E-04	2.0E-04	5.5E-05	3.9E+01	5
3.0E-01	2.0E-01	4.0E-01			2
2.0E-01					1

Table 10. continued

compound class	carbon #	compound
Other (continued)	12	Dibenzothiophene
	13	1-Methylcarbazole
	13	2-Methylcarbazole
	13	3-Methylcarbazole
	13	4-Methylcarbazole
	14	1,2-Dimethylcarbazole
	14	1,3-Dimethylcarbazole
	14	1,4-Dimethylcarbazole
	14	1,6-Dimethyldibenzothiophene
	14	2,6-Dimethyldibenzothiophene and 2-Ethyldibenzothiophene
	14	2-Phenylindole
	15	6-Phenylquinoline
	16	2-Ethyldibenzothiophene
	16	Benzo[def]carbazole
	18	9-Phenylcarbazole
Polynuclear Aromatics		Total Acenaphthenes
		Total Acenaphthylenes
		Total Biphenyls and Acenaphthenes
		Total Phenanthrenes
		Total Triaromatics
	14	2-Aminoanthracene
	14	2-Aminophenanthrene
	14	3-Aminophenanthrene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.5E-02	1.3E-02	1.7E-02	2.1E-03	1.4E+01	5
1.6E-03	9.0E-04	2.1E-03	6.0E-04	3.7E+01	5
4.8E-04	2.0E-04	8.0E-04	2.4E-04	5.0E+01	5
3.8E-04	1.0E-04	6.0E-04	1.9E-04	5.1E+01	5
7.6E-04	3.0E-04	1.0E-03	3.4E-04	4.4E+01	5
5.8E-04	2.0E-04	8.0E-04	2.7E-04	4.6E+01	5
3.4E-04	1.0E-04	6.0E-04	1.9E-04	5.7E+01	5
1.0E-03	1.6E-04	1.9E-03	7.6E-04	7.5E+01	5
6.7E-03	2.5E-03	1.3E-02	4.0E-03	6.0E+01	5
2.0E-02	1.3E-02	3.2E-02	7.7E-03	3.9E+01	5
3.8E-04	2.0E-04	5.0E-04	1.3E-04	3.4E+01	5
7.0E-04	4.0E-04	1.1E-03	2.5E-04	3.6E+01	5
1.7E-02	1.3E-03	3.2E-02	1.1E-02	6.5E+01	5
3.0E-04	1.0E-04	5.0E-04	1.4E-04	4.7E+01	5
3.6E-04	1.0E-04	6.0E-04	1.8E-04	5.0E+01	5
1.9E+00	6.0E-02	5.4E+00	1.5E+00	7.8E+01	24
1.5E+00	6.0E-04	3.9E+00	9.0E-01	5.8E+01	20
2.6E+00					1
3.1E-01	1.7E-02	7.0E-01	3.5E-01	1.1E+02	3
5.0E-01	7.0E-02	1.6E+00	5.0E-01	9.9E+01	10
4.0E-04	1.0E-04	5.0E-04	1.7E-04	4.3E+01	5
2.4E-04	1.0E-04	4.0E-04	1.1E-04	4.8E+01	5
2.0E-04	1.0E-04	3.0E-04	7.1E-05	3.5E+01	5

Table 10. continued

compound class	carbon #	compound
Polynuclear Aromatics (continued)	14	4-Aminophenanthrene
	14	Anthracene
	14	Phenanthrene
	15	1-Methylphenanthrene
	15	2-Methylanthracene
	15	2-Methylphenanthrene
	15	3-Methylphenanthrene
	15	4- & 9-Methylphenanthrene
	15	9-Cyanoanthracene
	15	9-Cyanophenanthrene
	15	Total Methylanthracenes
	15	Total Methylphenanthrenes
	16	Fluoranthene
	16	Pyrene
	16	Total Dimethylphenanthrenes
	17	1-Methylpyrene
	17	2-Methylpyrene
	17	Benzo(a)fluorene
	18	1-Methyl-7-isopropylphenanthrene
	18	Benz(a)anthracene
	18	Benzo(g,h,i)fluoranthene
	18	Chrysene
	18	Chrysene and Triphenylene
	18	Triphenylene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
3.4E-04	1.0E-04	6.0E-04	1.9E-04	5.7E+01	5
5.8E-03	3.0E-06	2.0E-02	7.5E-03	1.3E+02	14
8.8E-02	2.7E-05	3.0E-01	9.2E-02	1.1E+02	20
5.1E-03	1.1E-05	2.4E-02	8.0E-03	1.6E+02	8
5.3E-03	1.5E-05	1.8E-02	6.3E-03	1.2E+02	8
1.6E-01	1.4E-01	1.8E-01	1.3E-02	8.2E+00	6
3.8E-03	1.3E-05	1.1E-02	4.4E-03	1.2E+02	8
6.7E-03	1.3E-05	3.4E-02	1.1E-02	1.7E+02	8
6.4E-04	3.0E-04	9.0E-04	2.8E-04	4.4E+01	5
6.8E-04	4.0E-04	1.0E-03	2.8E-04	4.1E+01	5
9.3E-04					1
2.5E-01	1.6E-01	5.0E-01	1.3E-01	5.2E+01	6
5.9E-03	6.8E-07	2.0E-02	8.0E-03	1.4E+02	15
4.6E-03	1.8E-05	1.5E-02	6.0E-03	1.3E+02	15
5.7E-02	2.0E-02	2.1E-01	7.5E-02	1.3E+02	6
2.9E-04	2.4E-06	1.4E-03	4.7E-04	1.6E+02	8
2.8E-04	3.7E-06	1.1E-03	3.8E-04	1.3E+02	8
2.8E-04	5.4E-07	1.3E-03	4.3E-04	1.5E+02	8
6.6E-04	1.5E-06	4.0E-03	1.4E-03	2.0E+02	8
9.6E-05	2.0E-06	6.7E-04	2.2E-04	2.3E+02	9
9.3E-05	2.5E-07	3.5E-04	1.3E-04	1.4E+02	8
4.5E-05					1
1.2E-04	8.4E-07	4.9E-04	1.7E-04	1.4E+02	8
3.3E-04					1

Table 10. continued

compound class	carbon #	compound
Polynuclear Aromatics (continued)	20	Benzo(a)pyrene
	20	Benzo(b+k)fluoranthene
	20	Benzo(e)pyrene
	21	Cyclopenta(cd)pyrene
	22	Benzo(g,h,i)perylene
	22	Indeno(1,2,3-cd)pyrene
	22	Picene
Total Aromatics		Total Aromatics
		Total Aromatics by HPLC
Total Cycloalkanes		Total Cycloalkanes
Total Diaromatics (IncludingNaphthalenes)		Total Diaromatics (Including Naphthalenes)
Total Monoaromatics		Total Monoaromatics
Total n-Alkanes		Total n-Alkanes
Total Polynuclear Aromatics		Total Polynuclear Aromatics
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes
		Total Straight-Chain and Branched Alkanes by HPLC

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
2.2E-04	5.0E-06	8.4E-04	3.5E-04	1.6E+02	5
3.1E-05	3.1E-07	1.9E-04	6.7E-05	2.1E+02	8
3.8E-05	5.4E-06	2.4E-04	7.6E-05	2.0E+02	9
6.8E-05	1.6E-06	3.7E-04	1.2E-04	1.8E+02	8
1.2E-05	9.1E-07	4.0E-05	1.6E-05	1.4E+02	8
1.6E-05	6.4E-07	9.7E-05	3.3E-05	2.0E+02	8
1.5E-05	3.5E-07	8.3E-05	3.0E-05	2.0E+02	7
2.2E+01	2.0E+00	3.9E+01	8.6E+00	3.8E+01	28
2.3E+01	8.7E+00	3.8E+01	8.0E+00	3.5E+01	19
3.7E+01	5.3E+00	5.4E+01	9.9E+00	2.6E+01	28
6.3E+00	7.3E-02	2.0E+01	4.4E+00	7.0E+01	27
1.6E+01	3.7E+00	2.2E+01	5.1E+00	3.2E+01	26
1.3E+01	9.4E+00	3.3E+01	4.9E+00	3.7E+01	19
3.6E-01	1.5E-04	2.3E+00	7.6E-01	2.1E+02	10
4.1E+01	2.5E+01	7.5E+01	9.9E+00	2.4E+01	29
6.4E+01	5.1E+01	7.6E+01	6.7E+00	1.0E+01	19

Table 11. Summary of Composition Data for No. 2 Fuel Oil

compound class	carbon #	compound
Alkenes		Total Alkenes
Alkyl-Monoaromatics		Total Alkyl-Monoaromatics
	7	Toluene
	8	Ethylbenzene
	8	Total Xylenes
Cycloalkanes		Total Dicycloalkanes
		Total Monocycloalkanes
		Total Tricycloalkanes
Diaromatics (Except Naphthalenes)		Total Fluorenes and Acenaphthylenes
	12	Biphenyl
	13	Fluorene
	14	Total Methylfluorenes
	15	Total Dimethylfluorenes
	16	Total Trimethylfluorenes
Metals		Nickel
		Vanadium
Monoaromatics		Total Dinaphthenobenzenes
		Total Dinaphthenobenzenes and Indenes
		Total Indenes
	9	Indene
	10	Total Indans and Tetralins
n-Alkanes		n-Decane and n-Undecane
	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
2.0E+00					1
6.9E+00	5.2E+00	1.0E+01	2.0E+00	2.8E+01	6
6.2E-02	2.5E-02	1.1E-01	4.4E-02	7.1E+01	3
3.4E-02	2.8E-02	4.0E-02			2
2.3E-01	1.5E-01	4.3E-01	1.3E-01	5.8E+01	4
7.2E+00	4.2E+00	9.4E+00	1.8E+00	2.6E+01	6
1.1E+01	5.0E+00	1.8E+01	5.7E+00	5.3E+01	6
1.8E+00	5.8E-01	4.5E+00	1.4E+00	8.0E+01	6
1.1E+00	4.4E-01	2.0E+00	8.2E-01	7.3E+01	3
7.2E-03	5.9E-03	8.6E-03			2
1.9E-02	4.3E-03	4.5E-02	1.9E-02	1.0E+02	4
1.5E-02	1.5E-02	1.5E-02			2
3.1E-02	2.7E-02	3.5E-02			2
2.8E-02	1.9E-02	3.6E-02			2
5.0E-05					1
1.5E-04					1
4.6E+00					1
1.5E+00	1.3E+00	1.8E+00	2.5E-01	1.6E+01	3
1.1E+00	1.0E+00	1.3E+00			2
1.9E-02	8.7E-03	2.9E-02			2
5.0E+00	4.1E+00	7.3E+00	1.2E+00	2.4E+01	6
1.3E+00					1
1.0E-01	1.0E-01	1.0E-01			2
3.0E-01	3.0E-01	3.0E-01			2
5.0E-01	5.0E-01	5.0E-01			2
8.5E-01	8.0E-01	9.0E-01			2
1.1E+00	8.4E-01	1.2E+00	2.1E-01	1.9E+01	3
1.6E+00	9.6E-01	2.0E+00	5.7E-01	3.5E+01	3
2.0E+00	1.0E+00	2.5E+00	8.2E-01	4.2E+01	3
2.4E+00	1.1E+00	3.2E+00	1.1E+00	4.6E+01	3
2.4E+00	1.0E+00	3.3E+00	1.2E+00	5.0E+01	3

Table 11. continued

compound class	carbon #	compound
n-Alkanes (continued)	17	n-Heptadecane
	18	n-Octadecane
	19	n-Nonadecane
	20	n-Eicosane
	21	n-Heneicosane
	22	n-Docosane
Naphthalenes		Total Naphthalenes
	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	11	Total Methylnaphthalenes
	12	1,4-Dimethylnaphthalene
	12	Total Dimethylnaphthalenes
	13	Total Trimethylnaphthalenes
	14	Total Tetramethylnaphthalenes
Other	8	Total Benzothiophenes
	12	Dibenzothiophene
	13	Total Methyldibenzothiophenes
	14	Total Dimethyldibenzothiophenes
	15	Total Trimethyldibenzothiophenes
Polynuclear Aromatics		Total Acenaphthalenes
		Total Acenaphthenes
		Total Biphenyls and Acenaphthenes
		Total Methylfluoranthenes and Pyrenes
		Total Phenanthrenes
		Total Tricyclicaromatics
	12	Acenaphthene
	12	Acenaphthylene
	14	Anthracene
	14	Phenanthrene
	15	1-Methylphenanthrene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
2.4E+00	6.5E-01	3.6E+00	1.6E+00	6.5E+01	3
1.8E+00	5.5E-01	2.5E+00	1.0E+00	6.0E+01	3
8.8E-01	3.3E-01	1.3E+00	5.0E-01	5.7E+01	3
3.6E-01	1.8E-01	6.0E-01	2.2E-01	6.0E+01	3
2.0E-01	9.0E-02	4.0E-01	1.8E-01	9.0E+01	3
1.0E-01					1
1.0E+01	8.5E+00	1.2E+01	1.8E+00	1.7E+01	3
2.2E-01	9.0E-03	4.0E-01	1.3E-01	6.1E+01	10
3.9E-01	2.9E-01	4.8E-01			2
6.8E-01	3.6E-01	1.0E+00	2.7E-01	3.9E+01	4
1.2E+00	6.4E-02	2.7E+00	1.4E+00	1.1E+02	4
4.4E-02	4.3E-02	4.5E-02			2
1.7E+00	1.5E-01	3.2E+00	1.7E+00	1.0E+02	4
6.9E-01	1.1E-01	1.8E+00	1.0E+00	1.5E+02	3
3.3E-01	6.3E-02	5.9E-01			2
9.0E-01					1
1.7E-02					1
4.9E-03	2.5E-03	7.4E-03			2
9.4E-03	9.1E-03	9.6E-03			2
8.7E-03	7.1E-03	1.0E-02			2
2.1E+00	3.0E-01	5.4E+00	2.9E+00	1.4E+02	3
2.1E+00	1.1E+00	3.8E+00	1.5E+00	7.0E+01	3
1.9E+00	1.6E+00	2.3E+00			2
5.4E-03	1.7E-03	9.1E-03			2
6.7E-01	2.9E-01	1.0E+00	3.7E-01	5.5E+01	3
3.0E-01	2.0E-01	4.0E-01			2
1.8E-02	1.3E-02	2.2E-02			2
6.0E-03					1
2.8E-03	1.0E-04	1.1E-02	4.3E-03	1.5E+02	6
7.9E-02	9.1E-03	1.7E-01	5.3E-02	6.7E+01	10
1.7E-02					1

Table 11. continued

compound class	carbon #	compound
Polynuclear Aromatics (continued)	15	2-Methylanthracene
	15	2-Methylphenanthrene
	15	Methylanthracene
	15	Total Methylphenanthrenes
	16	9,10-Dimethylanthracene
	16	Fluoranthene
	16	Pyrene
	16	Total Dimethylphenanthrenes
	17	Total Trimethylphenanthrenes
	18	Benz(a)anthracene
	18	Chrysene
	18	Total Tetramethylphenanthrenes
	18	Triphenylene
	19	Total Methylchrysenes
	20	Benzo(a)pyrene
	20	Benzo(e)pyrene
	20	Benzo(g,h,i)pyrene
	20	Total Dimethylchrysenes
	21	Total Trimethylchrysenes
	22	Benzo(g,h,i)perylene
Total Aromatics		Total Aromatics
Total Branched Alkanes		Total Branched Alkanes
Total n-Alkanes		Total n-Alkanes
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.3E-02	9.1E-03	1.7E-02			2
7.7E-01	7.7E-01	7.7E-01			2
1.6E-03	6.6E-04	2.1E-03	6.7E-04	4.2E+01	4
2.9E-01	4.2E-02	7.9E-01	4.2E-01	1.4E+02	3
3.9E-03	1.8E-03	6.0E-03			2
1.4E-03	4.7E-05	3.7E-03	1.5E-03	1.1E+02	9
2.9E-03	4.5E-05	1.2E-02	3.8E-03	1.3E+02	9
8.1E-02	5.4E-02	1.1E-01			2
5.1E-02	2.2E-02	8.0E-02			2
4.5E-05	2.0E-06	1.2E-04	5.5E-05	1.2E+02	8
1.4E-04	3.7E-05	3.9E-04	1.3E-04	9.2E+01	8
2.1E-02	8.7E-03	3.2E-02			2
1.0E-04	2.3E-05	1.4E-04	5.0E-05	5.0E+01	5
3.9E-04	9.1E-05	6.8E-04			2
2.1E-05	1.0E-06	6.0E-05	2.7E-05	1.3E+02	7
5.2E-06	2.0E-06	1.0E-05	4.4E-06	8.4E+01	5
2.8E-06	1.0E-06	7.0E-06	2.9E-06	1.0E+02	4
2.3E-04	4.6E-05	4.2E-04			2
9.5E-05	9.1E-06	1.8E-04			2
5.7E-06					1
2.7E+01	1.8E+01	3.8E+01	7.5E+00	2.8E+01	6
2.2E+01					1
1.7E+01	8.1E+00	2.1E+01	7.5E+00	4.5E+01	3
5.4E+01	3.4E+01	6.6E+01	1.1E+01	2.0E+01	7

Table 12. Summary of Composition Data for No.6 Fuel Oil

compound class	carbon #	compound
Alkyl-Monoaromatics		Total Alkyl-Monoaromatics
Branched Alkanes	19	Pristane
	20	Phytane
Cycloalkanes		Total Dicycloalkanes
		Total Hexacycloalkanes
		Total Monocycloalkanes
		Total Pentacycloalkanes
		Total Tetracycloalkanes
		Total Tricycloalkanes
Metals		Nickel
		Vanadium
Monoaromatics	10	Total Indans and Tetralins
n-Alkanes		Total n-alkanes n-C32 and larger
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
	18	n-Octadecane
	19	n-Nonadecane
	20	n-Eicosane
	21	n-Heneicosane
	22	n-Docosane
	23	n-Tricosane
	24	n-Tetracosane
	25	n-Pentacosane
	26	n-Hexacosane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.9E+00					1
5.1E-02	4.1E-02	6.2E-02			2
6.3E-02	5.5E-02	7.1E-02			2
3.4E+00					1
4.0E-01					1
3.9E+00					1
1.9E+00					1
2.7E+00					1
2.9E+00					1
8.9E-03					1
7.3E-03					1
2.1E+00					1
5.0E-02					1
3.4E-03	9.0E-04	5.9E-03			2
8.8E-03	2.7E-03	1.5E-02			2
1.5E-02	5.7E-03	2.5E-02			2
2.2E-02	1.0E-02	3.4E-02			2
4.3E-02	1.7E-02	7.0E-02	2.7E-02	6.2E+01	3
6.3E-02	2.4E-02	1.1E-01	4.4E-02	6.9E+01	3
7.3E-02	3.0E-02	1.2E-01	4.5E-02	6.2E+01	3
9.0E-02	4.4E-02	1.4E-01	4.8E-02	5.4E+01	3
1.0E-01	5.6E-02	1.5E-01	4.7E-02	4.6E+01	3
8.8E-02	4.1E-02	1.2E-01	4.2E-02	4.7E+01	3
1.0E-01	5.5E-02	1.4E-01	4.3E-02	4.3E+01	3
1.0E-01	6.0E-02	1.2E-01	3.4E-02	3.4E+01	3
1.0E-01	6.4E-02	1.3E-01	3.4E-02	3.3E+01	3
1.0E-01	6.8E-02	1.4E-01	3.4E-02	3.3E+01	3
9.6E-02	6.7E-02	1.3E-01	3.3E-02	3.4E+01	3
9.3E-02	6.7E-02	1.3E-01	3.4E-02	3.6E+01	3
8.2E-02	6.2E-02	1.1E-01	2.8E-02	3.4E+01	3
7.1E-02	5.0E-02	1.0E-01	2.9E-02	4.0E+01	3

Table 12. continued

compound class	carbon #	compound
n-Alkanes (continued)	27	n-Heptacosane
	28	n-Octacosane
	29	n-Nonacosane
	30	n-Triacontane
	31	n-Hentricontane
	32	n-Dotriacontane
	33	n-Tritriacontane
	34	n-Tetratriacontane
	35	n-Pentatriacontane
	36	n-Hexatriacontane
	37	n-Heptatriacontane
	38	n-Octatriacontane
	39	n-Nonatriacontane
	40	n-Tetracontane
Naphthalenes		Total Naphthalenes
	10	Naphthalene
	11	Total Methylnaphthalenes
Other		Asphaltenes and Polars
		Insolubles
		Polar Materials
	12	Total Dibenzothiophenes
Polynuclear Aromatics		Total Chrysenes
		Total Fluoranthenes
		Total Phenanthrenes
	14	Anthracene
	14	Phenanthrene
	15	1-Methylphenanthrene
	15	2-Methylphenanthrene
	16	Fluoranthene
	16	Pyrene
	18	Benz(a)anthracene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
6.6E-02	4.0E-02	9.9E-02	3.0E-02	4.6E+01	3
6.6E-02	5.0E-02	9.2E-02	2.3E-02	3.5E+01	3
5.8E-02	4.0E-02	8.5E-02	2.3E-02	4.0E+01	3
5.3E-02	4.0E-02	7.5E-02	2.0E-02	3.7E+01	3
4.6E-02	3.7E-02	6.0E-02	1.2E-02	2.7E+01	3
4.1E-02	3.2E-02	5.1E-02			2
3.1E-02	2.6E-02	3.6E-02			2
2.6E-02	2.2E-02	3.0E-02			2
1.5E-02	1.5E-02	1.5E-02			2
1.1E-02	1.1E-02	1.1E-02			2
9.6E-03	9.2E-03	9.9E-03			2
7.7E-03	6.6E-03	8.7E-03			2
6.2E-03	4.8E-03	7.6E-03			2
4.8E-03	4.2E-03	5.5E-03			2
9.8E-02	4.0E-04	9.2E-01	2.6E-01	2.7E+02	12
4.2E-03	2.1E-04	1.5E-02	7.0E-03	1.7E+02	4
2.6E+00					1
5.8E+00	7.0E-02	2.5E+01	7.8E+00	1.3E+02	12
1.4E+01					1
3.0E+01					1
9.8E-02	2.0E-04	7.0E-01	1.8E-01	1.9E+02	13
1.8E-02	2.3E-03	2.7E-02	7.0E-03	4.0E+01	12
1.8E-02	3.0E-04	3.3E-02	1.1E-02	6.4E+01	12
6.6E-02	1.3E-03	1.5E-01	5.0E-02	7.6E+01	13
5.0E-03					1
2.1E-02	2.1E-03	4.8E-02	2.4E-02	1.2E+02	5
4.3E-03					1
8.3E-02					1
2.4E-02					1
2.3E-03					1
5.5E-02	2.9E-03	1.5E-01	8.4E-02	1.5E+02	3

Table 12. continued

compound class	carbon #	compound
Polynuclear Aromatics (continued)	18	Chrysene
	18	Triphenylene
	20	Benzo(a)pyrene
	20	Benzo(b+k)fluoranthene
	20	Benzo(e)pyrene
	20	Perylene
	22	Indeno(1,2,3-cd)pyrene
Total Aromatics		Total Aromatics
Total n-Alkanes		Total n-Alkanes
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
6.9E-02	2.9E-03	3.1E-01	1.3E-01	2.0E+02	5
3.1E-03					1
4.4E-03					1
4.4E-02					1
1.0E-03					1
2.2E-03					1
1.0E-02					1
3.4E+01					1
1.7E+00					1
1.3E+01	5.0E+00	2.1E+01			2

Table 13. Summary of Composition Data for Lubricating and Motor Oils

compound class	carbon #	compound
Alkyl-Monoaromatics		Total Alkyl-Monoaromatics
	6	Benzene
	7	Toluene
	8	Total Xylenes
Branched Alkanes	10	trans-Decalin
	19	Pristane
	20	Phytane
Chlorinated Solvents	1	Dichlorodifluoromethane
	2	1,1,1-Trichloroethane
	2	Tetrachloroethylene (PCE)
	2	Trichloroethylene (TCE)
	2	Trichlorotrifluoroethane
Cycloalkanes		Total Dicycloalkanes
		Total Hexacycloalkanes
		Total Monocycloalkanes
		Total Pentacycloalkanes
		Total Tetracycloalkanes
		Total Tricycloalkanes
	15	Nonylcyclohexane
	16	Octylcyclohexane
Diaromatics (Except Naphthalenes)		TotalBiphenyls/Acenapthenes/Fluorenes
		Total Fluorenes
	12	Biphenyl
	13	4-Phenyltoluene
	13	Fluorene
	13	Total Methylbiphenyls
	14	Total Methylfluorenes
	15	Total Dimethylfluorenes
	16	Total Trimethylfluorenes
Inorganics		Total Chlorine
Metals		Arsenic
		Barium
		Cadmium
		Chromium

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
4.2E+00	1.0E-01	8.4E+00			2
9.6E-02	5.9E-02	9.6E-02			237
2.2E-01	1.0E-01	2.2E-01			243
3.4E-01	2.0E-01	3.4E-01			236
1.0E-03					1
2.0E-02	1.2E-02	2.8E-02			2
2.7E-02	1.8E-02	3.7E-02			2
3.7E-02					87
2.8E-01	4.0E-02	2.8E-01			617
1.4E-01	1.8E-02	1.4E-01			600
1.4E-01	2.5E-04	1.4E-01			609
6.3E+00					28
1.0E+01					1
1.9E+00					1
7.0E+00					1
3.7E+00					1
5.9E+00					1
6.6E+00					1
1.5E-03	9.0E-04	2.2E-03			2
1.1E-03	1.0E-03	1.1E-03			2
6.4E+00					1
3.4E-03					1
6.4E-03	4.6E-03	8.3E-03			2
4.0E-04	2.0E-04	6.0E-04			2
4.5E-03	1.7E-04	1.1E-02	5.3E-03	1.2E+02	5
2.3E-04					1
2.8E-04					1
1.4E-04					1
1.3E-04					1
5.0E-01	1.2E-01	5.0E-01			591
1.7E-03	1.0E-03	1.7E-03			538
1.3E-02	1.3E-02	2.1E-02			753
3.1E-04	1.7E-04	3.1E-04			745
2.8E-03	1.1E-04	2.8E-03			757

Table 13. continued

compound class	carbon #	compound
Metals (continued)		Lead
		Zinc
Monoaromatics	10	Tetralin
	14	Total Napthenobenzenes
n-Alkanes	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
	18	n-Octadecane
	19	n-Nonadecane
	20	n-Eicosane
Naphthalenes		Total Naphthalenes
	10	Naphthalene
	11	1-Methylnaphthalene
	11	Total Methylnaphthalenes
	12	1,5-Dimethylnaphthalene
	12	2-Ethylnaphthalene
	12	Total Dimethylnaphthalenes
	13	1,3,5-Trimethylnaphthalene
Other		Total Polychlorinated Biphenyls (PCB's)
		Total Sulfur Containing Heterocyclics
	12	Dibenzothiophene
	13	Total Methyldibenzothiophenes
	14	Total Dimethyldibenzothiophenes
	15	Total Trimethyldibenzothiophenes
	16	Benzo(b)naptho(2,1-d)thiophene
	16	Benzonaphthothiophene
	16	Other Benzonaphthothiophenes
	16	Phenanthro(4,4a,4b,5-bcd)thiophene
	16	Total Benzonaphthofurans
	17	Total Methylbenzonaphthothiophenes

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
6.7E-02	6.6E-02	2.6E-01			836
5.8E-02	5.8E-02	9.8E-02			811
1.2E-03	7.0E-05	2.4E-03			2
9.8E+00					1
1.4E-02					1
1.3E-02	2.6E-03	2.3E-02			2
1.4E-02	1.3E-02	1.5E-02			2
1.3E-02	1.2E-02	1.4E-02			2
2.1E-02	1.4E-02	2.8E-02			2
3.7E-02	2.2E-02	5.3E-02			2
5.1E-02	3.7E-02	6.4E-02			2
7.4E-02	6.7E-02	8.2E-02			2
2.0E-01	1.8E-01	2.2E-01			2
3.2E+00	5.0E-02	6.4E+00			2
5.9E-02	5.0E-05	2.5E-01	1.3E-01	1.0E+02	29
3.0E-03	2.0E-04	5.7E-03			2
5.2E-01	4.1E-01	6.3E-01			2
2.9E-03	3.0E-04	5.6E-03			2
3.0E-03	2.0E-04	5.8E-03			2
3.7E-01	3.0E-01	4.5E-01			2
2.0E-03	4.0E-04	3.7E-03			2
1.1E-02	3.9E-03	1.1E-02			754
2.3E-03					1
9.0E-05					1
2.6E-04					1
4.4E-04					1
2.2E-04					1
3.8E-04	1.9E-04	4.8E-04	8.6E-05	2.9E+01	81
3.9E-05					1
1.4E-04					1
4.1E-05					1
5.1E-05					1
6.2E-05					1

Table 13. continued

compound class	carbon #	compound
Other (continued)	22	Triphenylene(4,4a,4b,5-bcd)thiophene
Polynuclear Aromatics		Terphenyl
		Total Benzanthracenes/Chrysenes/ Triphenylenes
		Total Fluoranthenes
		Total Perylenes
		Total Phenanthrenes
	14	Anthracene
	14	Phenanthrene
	15	Total Methylanthracenes
	15	Total Methylphenanthrenes
	16	Fluoranthene
	16	Phenylnaphthalene
	16	Pyrene
	16	Total Dimethylanthracenes
	16	Total Dimethylphenanthrenes
	17	1-Methylpyrene
	17	4-Methylpyrene
	17	Benzo(a)fluorene
	17	Benzo(b)fluorene
	17	Benzo(c)fluorene
	17	TotalBenzofluorenes
	17	Total Dihydromethylpyrenes
	17	Total Methylpyrenes
	17	Total Trimethylanthracenes
	17	Total Trimethylphenanthrenes
	18	Benz(a)anthracene
	18	Benzo(c)phenanthrene
	18	Chrysene
	18	Chrysene and Triphenylene
	18	Total Chrysenes and Benzanthracenes
	18	Total Chrysenes and Triphenylenes
	18	Total Diethylphenanthrenes
	18	Total Dimethylpyrenes

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.2E-05					1
1.4E-05					1
3.4E-03					1
6.8E-03					1
1.0E+00					1
3.7E+00	2.5E-02	7.4E+00			2
2.2E-03	3.8E-05	4.7E-03	2.1E-03	9.6E+01	4
7.9E-03	4.0E-04	1.9E-02	8.7E-03	1.1E+02	6
6.6E-05					1
4.4E-02	1.3E-03	6.7E-02	3.7E-02	8.4E+01	3
3.8E-03	7.0E-05	9.1E-03	3.3E-03	1.3E+02	86
1.0E-04					1
1.0E-02	1.7E-04	1.6E-02	3.7E-03	1.4E+02	86
3.0E-05					1
1.2E-03					1
1.3E-04					1
1.9E-04					1
1.9E-04	1.1E-04	2.7E-04			2
1.6E-04					1
5.0E-05					1
3.8E-04					1
5.1E-05					1
4.8E-04					1
5.8E-05					1
6.9E-04					1
6.3E-03	3.4E-05	7.1E-03	2.2E-03	1.4E+02	32
1.4E-05					1
3.5E-03	1.3E-04	8.5E-03	4.0E-03	1.2E+02	4
1.4E-03	2.4E-04	3.4E-03	1.3E-03	9.0E+01	5
2.2E+00					1
2.8E-03	2.8E-04	3.8E-03			77
1.4E-04					1
1.9E-04					1

Table 13. continued

compound class	carbon #	compound
Polynuclear Aromatics (continued)	18	Triphenylene
	19	Total Ethylmethylpyrenes
	19	Total Methylbenzo(a)anthracenes
	20	Benzo(a)pyrene
	20	Benzo(b)fluoranthene
	20	Benzo(e)pyrene
	20	Benzo(k)fluoranthene
	20	Ethylbenz(a)anthracene
	20	Perylene
	20	Total Benzofluoranthenes (b+j+k)
	20	Total Benzpyrenes and Benzfluoranthenes
	21	Cyclopenta(cd)pyrene
	21	Methylbenzo(mno)fluoranthene
	21	Total Ethylcyclopenta(def)phenanthrenes
	21	Total Methylbenzo(e)pyrenes
	21	Total Methylbenzofluoranthenes
	21	Total Methylbenzopyrenes
	22	Benzo(g,h,i)perylene
	22	Dibenz(a,c)anthracene
	22	Indeno(1,2,3-cd)pyrene
	24	Coronene
	24	Total Benzperylenes
Total Aromatics		Total Aromatics
Total Cycloalkanes		Total Cycloalkanes
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
2.5E-04					1
1.6E-05					1
2.8E-04					1
1.7E-03	3.0E-06	2.5E-03	7.1E-04	1.8E+02	151
4.0E-05	3.7E-05	4.3E-05			2
1.7E-03	2.2E-05	3.1E-03	1.3E-03	1.5E+02	84
6.1E-05	4.0E-06	1.6E-04	8.6E-05	1.4E+02	3
7.4E-05					1
3.5E-04	8.0E-06	5.1E-04	2.0E-04	1.9E+02	82
1.5E-03	1.2E-05	2.6E-03	1.1E-03	1.4E+02	81
2.5E-03					1
8.9E-05					1
3.4E-05					1
1.6E-04					1
2.6E-05					1
2.1E-05					1
4.7E-05					1
2.8E-03	7.0E-06	4.8E-03	1.7E-03	2.4E+02	84
8.0E-06					1
4.0E-03	1.1E-06	6.1E-03	3.1E-04	1.7E+02	82
7.0E-05	8.5E-07	1.7E-03	7.2E-04	1.9E+02	27
2.7E-03					1
2.2E+01	2.0E-01	4.5E+01	2.2E+01	1.0E+02	3
2.9E+01					1
4.4E+01	1.7E+01	6.1E+01	2.3E+01	5.3E+01	3

Table 14. Summary of Composition Data for Crude Oil

compound class	carbon #	compound
Alkyl-Monoaromatics	6	Benzene
	7	Toluene
	8	1,2-Diethylbenzene
	8	Ethylbenzene
	8	m+p-Xylenes
	8	m-Xylene
	8	o-Xylene
	8	p-Xylene
	9	1,2,3-Trimethylbenzene
	9	1,2,4-Trimethylbenzene
	9	1,3,5-Trimethylbenzene
	9	1-Methyl-2-ethylbenzene
	9	1-Methyl-3-ethylbenzene
	9	1-Methyl-4-ethylbenzene
	9	Isopropylbenzene
	9	n-Propylbenzene
	10	1,2,3,5-Tetramethylbenzene
	10	1,2,4,5-Tetramethylbenzene
	10	1,2-Dimethyl-4-ethylbenzene
	10	1,3-Dimethyl-5-ethylbenzene
	10	1-Methyl-4-isopropylbenzene
	10	Indane
	10	sec-Butylbenzene
	10	tert-Butylbenzene
Branched Alkanes	6	2,2-Dimethylbutane
	6	2,3-Dimethylbutane
	6	2-Methylpentane
	6	3-Methylpentane
	7	2,3-Dimethylpentane
	7	2,4-Dimethylpentane
	7	2-Methylhexane
	7	3-Ethylpentane
	7	3-Methylhexane

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
1.6E-01	4.0E-02	4.1E-01	1.3E-01	7.9E+01	8
6.7E-01	8.2E-02	2.5E+00	7.1E-01	1.1E+02	9
2.4E-02					1
1.7E-01	5.6E-02	3.1E-01	8.4E-02	5.0E+01	9
5.0E-01	2.0E-01	8.0E-01			2
6.6E-01	8.0E-02	2.0E+00	6.3E-01	9.6E+01	7
2.6E-01	3.0E-02	6.8E-01	1.9E-01	7.1E+01	9
2.6E-01	9.0E-02	6.8E-01	2.4E-01	9.1E+01	8
1.0E-01					1
2.4E-01	5.0E-02	5.1E-01	1.7E-01	7.1E+01	8
1.8E-01	4.1E-02	6.9E-01	2.0E-01	1.1E+02	9
5.0E-02	1.0E-02	9.0E-02	3.3E-02	6.5E+01	7
1.4E-01	1.0E-02	4.0E-01	1.3E-01	9.1E+01	7
6.0E-02	3.0E-02	1.3E-01	3.4E-02	5.7E+01	7
4.4E-02	1.6E-02	9.0E-02	2.4E-02	5.5E+01	9
8.6E-02	2.0E-02	2.6E-01	7.8E-02	9.0E+01	8
2.7E-02					1
3.8E-02					1
2.4E-02					1
2.7E-02					1
1.2E-02					1
6.7E-02					1
1.4E-02					1
6.2E-03	2.0E-03	1.0E-02	4.2E-03	6.8E+01	6
4.2E-02	4.0E-02	4.3E-02			2
1.1E-01	8.0E-02	1.4E-01			2
3.7E-01	3.5E-01	4.0E-01			2
3.6E-01	3.0E-01	4.2E-01			2
3.5E-01	1.0E-01	6.0E-01			2
4.9E-02					1
7.0E-01					1
5.0E-02					1
3.4E-01	1.9E-01	5.0E-01			2

Table 14. continued

compound class	carbon #	compound
Branched Alkanes (continued)	8	2,2,3-Trimethylpentane
	8	2,2-Dimethylhexane
	8	2,3,3-Trimethylpentane
	8	2,3,4-Trimethylpentane
	8	2,3-Dimethylhexane
	8	2,4-Dimethylhexane
	8	2,5-Dimethylhexane
	8	2-Methyl-3-heptane
	8	3,3-Dimethylhexane
	8	Ethylcyclohexane
	9	2,3-Dimethylheptane
	9	2,6-Dimethylheptane
	9	2-Methyloctane
	9	3-Methyloctane
	9	4-Methyloctane
	19	Pristane
	20	Phytane
Cycloalkanes	5	Cyclopentane
	6	Cyclohexane
	6	Methylcyclopentane
	7	1,1-Dimethylcyclopentane
	7	cis-1,3-Dimethylcyclopentane
	7	Ethylcyclopentane
	7	trans-1,2-Dimethylcyclopentane
	7	trans-1,3-Dimethylcyclopentane
	8	1,1,2-Trimethylcyclopentane
	8	1,1,3-Trimethylcyclopentane
	8	trans-1,2-cis-4-Trimethylcyclopentane
	8	trans-1,2-Dimethylcyclohexane
	9	trans-1,2,4-Trimethylcyclohexane
Diaromatics (Except Naphthalenes)	12	Biphenyl
	13	Fluorene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
4.0E-03					1
6.4E-02	1.0E-02	1.2E-01			2
6.0E-03					1
5.0E-03					1
1.1E-01	6.0E-02	1.6E-01			2
6.0E-02					1
7.7E-02	6.0E-02	9.5E-02			2
4.0E-02					1
3.0E-02					1
2.0E-01					1
5.0E-02					1
1.5E-01	5.0E-02	2.5E-01			2
4.0E-01					1
2.6E-01	1.0E-01	4.2E-01			2
1.0E-01					1
2.1E-01					1
1.0E-01					1
4.8E-02	4.6E-02	5.0E-02			2
7.0E-01					1
6.0E-01	3.0E-01	9.0E-01			2
1.3E-01	6.3E-02	2.0E-01			2
2.0E-01					1
1.9E-01	1.9E-01	2.0E-01			2
3.3E-01	1.5E-01	5.0E-01			2
5.7E-01	2.4E-01	9.0E-01			2
6.0E-02					1
2.5E-01	2.0E-01	3.0E-01			2
3.3E-01	3.0E-01	3.6E-01			2
2.6E-01					1
2.0E-01	2.0E-01	2.0E-01			2
4.0E-02					1
2.0E-02	5.9E-03	6.0E-02	2.7E-02	1.3E+02	4

Table 14. continued

compound class	carbon #	compound
Monoaromatics	10	Tetralin
n-Alkanes	6	n-Hexane
	7	n-Heptane
	8	n-Octane
	9	n-Nonane
	10	n-Decane
	11	n-Undecane
	12	n-Dodecane
	13	n-Tridecane
	14	n-Tetradecane
	15	n-Pentadecane
	16	n-Hexadecane
	17	n-Heptadecane
	18	n-Octadecane
	19	n-Nonadecane
	20	n-Eicosane
	21	n-Heneicosane
	22	n-Docosane
	23	n-Tricosane
	24	n-Tetracosane
	25	n-Pentacosane
	26	n-Hexacosane
Naphthalenes	10	Naphthalene
	11	1-Methylnaphthalene
	11	2-Methylnaphthalene
	11	5-Methyltetralin
	11	6-Methyltetralin
	12	1,2-Dimethylnaphthalene
	12	1,3- & 1,6-Dimethylnaphthalene
	12	1,3-Dimethylnaphthalene
	12	1,4- & 2,3- & 1,5-Dimethylnaphthalene
	12	1,4-Dimethylnaphthalene
	12	1,5-Dimethylnaphthalene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
9.0E-02					1
1.3E+00	7.2E-01	1.8E+00			2
1.6E+00	8.5E-01	2.3E+00			2
1.1E+00	4.2E-01	1.9E+00	7.5E-01	7.0E+01	3
9.4E-01	4.4E-01	1.8E+00	7.5E-01	7.9E+01	3
1.1E+00	4.4E-01	1.8E+00			2
1.1E+00	4.7E-01	1.7E+00			2
1.1E+00	4.6E-01	1.7E+00			2
4.5E-01					1
4.2E-01					1
4.0E-01					1
3.7E-01					1
3.4E-01					1
2.5E-01					1
3.0E-01					1
1.9E-01					1
1.6E-01					1
1.9E-01					1
1.7E-01					1
1.3E-01					1
1.0E-01					1
7.6E-02					1
6.9E-02	3.3E-02	9.2E-02	2.8E-02	4.1E+01	4
1.3E-01	2.0E-02	3.1E-01	8.5E-02	6.3E+01	9
2.6E-01	9.3E-03	6.5E-01	1.9E-01	7.3E+01	9
8.0E-02					1
9.0E-02					1
3.7E-02	1.2E-02	7.4E-02	2.1E-02	5.7E+01	7
8.0E-02					1
1.1E-01	4.6E-02	2.1E-01	5.9E-02	5.6E+01	6
8.0E-02					1
2.4E-02	7.0E-03	6.8E-02	2.3E-02	9.9E+01	6
3.6E-02	1.1E-02	8.2E-02	2.7E-02	7.5E+01	6

Table 14. continued

compound class	carbon #	compound
Naphthalenes (continued)	12	1,6-Dimethylnaphthalene
	12	1,7-Dimethylnaphthalene
	12	1- & 2-Ethylnaphthalene
	12	1-Ethylnaphthalene
	12	2,3-Dimethylnaphthalene
	12	2,6- & 2,7-Dimethylnaphthalene
	12	2,6-Dimethylnaphthalene
	12	2,7-Dimethylnaphthalene
	12	2-Ethylnaphthalene
	13	1,2,4-Trimethylnaphthalene
	13	1,2,5-Trimethylnaphthalene
	13	1,2,6-Trimethylnaphthalene
	13	1,2,7-Trimethylnaphthalene
	13	1,3,5-Trimethylnaphthalene
	13	1,3,6-Trimethylnaphthalene
	13	1,3,7-Trimethylnaphthalene
	13	1,4,6- & 1,3,5-Trimethylnaphthalene
	13	1,4,6-Trimethylnaphthalene
	13	1,6,7-Trimethylnaphthalene
	13	2,3,6-Trimethylnaphthalene
Polynuclear Aromatics	12	Acenaphthene
	12	Acenaphthylene
	14	2-Methylfluorene
	14	Anthracene
	14	Phenanthrene
	15	1-Methylphenanthrene
	15	2-Methylphenanthrene
	15	3-Methylphenanthrene
	15	9-Methylphenanthrene
	16	1,6-Dimethylphenanthrene
	16	1,7-Dimethylphenanthrene
	16	1,8-Dimethylphenanthrene
	16	1,9-Dimethylphenanthrene

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
3.0E-01	1.4E-01	5.7E-01	1.7E-01	5.5E+01	6
1.1E-01	5.0E-02	2.1E-01	5.2E-02	4.7E+01	7
4.8E-02					1
3.4E-02	7.0E-03	8.5E-02	3.0E-02	9.0E+01	5
7.6E-02	2.7E-02	1.5E-01	4.5E-02	6.0E+01	6
6.9E-02					1
1.2E-01	5.4E-02	2.3E-01	6.0E-02	5.2E+01	6
1.4E-01	6.3E-02	2.8E-01	7.7E-02	5.5E+01	6
6.6E-02	2.1E-02	1.4E-01	4.1E-02	6.3E+01	6
3.0E-02	1.2E-02	5.6E-02	1.6E-02	5.4E+01	6
4.7E-02	1.9E-02	8.2E-02	2.4E-02	5.0E+01	6
4.2E-02	1.6E-02	7.7E-02	2.3E-02	5.5E+01	6
5.5E-02	2.1E-02	9.5E-02	2.7E-02	5.0E+01	6
2.6E-02	7.0E-03	4.9E-02	1.8E-02	6.7E+01	4
1.0E-01	4.3E-02	1.8E-01	5.1E-02	5.1E+01	6
6.7E-02	2.8E-02	1.2E-01	3.5E-02	5.2E+01	6
6.9E-02	4.0E-02	9.9E-02			2
5.3E-02	2.2E-02	9.5E-02	3.3E-02	6.2E+01	4
5.4E-02	2.3E-02	9.6E-02	2.8E-02	5.2E+01	6
4.9E-02	1.3E-02	8.7E-02	2.6E-02	5.3E+01	7
5.7E-03					1
1.3E-03					1
1.5E-02					1
1.1E-03					1
2.4E-02	2.6E-03	5.9E-02	1.7E-02	7.1E+01	13
1.3E-02	3.4E-03	3.3E-02	1.0E-02	7.7E+01	8
1.7E-02	6.1E-03	4.3E-02	1.2E-02	6.9E+01	8
1.6E-02	6.2E-03	3.7E-02	1.2E-02	7.1E+01	6
1.5E-02	4.8E-03	3.6E-02	1.2E-02	7.8E+01	6
8.8E-03	7.2E-03	1.0E-02			2
6.2E-03	1.6E-03	1.2E-02	3.7E-03	6.0E+01	6
1.2E-03	1.0E-04	3.0E-03	1.1E-03	9.1E+01	6
3.3E-03	7.0E-04	6.9E-03	2.2E-03	6.8E+01	6

Table 14. continued

compound class	carbon #	compound
Polynuclear Aromatics (continued)	16	2,3-Dimethylphenanthrene
	16	2,6-Dimethylphenanthrene
	16	2,7-Dimethylphenanthrene
	16	2,9-Dimethylphenanthrene
	16	3,6-Dimethylphenanthrene
	16	3,9-Dimethylphenanthrene
	16	9-Ethylphenanthrene
	16	Fluoranthene
	16	Pyrene
	17	1-Methylpyrene
	17	4-Methylpyrene
	18	Benz(a)anthracene
	18	Benzo(g,h,i)fluoranthene
	18	Chrysene
	18	Chrysene and Triphenylene
	18	Triphenylene
	19	2-Methylchrysene
	19	3-Methylchrysene
	19	4- & 6-Methylchrysene
	20	Benzo(a)pyrene
	20	Benzo(b)fluoranthene
	20	Benzo(e)pyrene
	20	Benzo(k)fluoranthene
	20	Perylene
	21	2-Methylcholanthene
	22	Benzo(g,h,i)perylene
	22	Indeno(1,2,3-cd)pyrene
	24	Coronene

*Summary statistics are a compilation of the data listed in the individual mixture composition data tables which are presented in Appendix I. All summary statistic values have units of %.

average wt %*	minimum*	maximum*	stdev*	coefficient of variation*	total number of data points
3.1E-03	7.0E-04	6.0E-03	1.9E-03	6.3E+01	6
7.6E-03	2.3E-03	1.4E-02	4.5E-03	5.9E+01	6
3.2E-03	9.0E-04	6.1E-03	1.9E-03	5.7E+01	6
7.8E-03	7.0E-03	8.5E-03			2
7.7E-03	5.6E-03	1.1E-02	2.9E-03	3.8E+01	3
8.6E-03	7.4E-03	9.7E-03			2
4.1E-03	1.4E-03	6.9E-03			2
3.9E-04	1.7E-04	6.0E-04	2.0E-04	5.0E+01	5
7.9E-04	3.5E-04	1.7E-03	5.8E-04	7.4E+01	5
2.5E-03	1.2E-03	3.9E-03			2
6.2E-04					1
3.2E-04	1.7E-04	6.7E-04	2.4E-04	7.4E+01	4
1.0E-04					1
1.3E-03	6.9E-04	1.8E-03	5.4E-04	4.2E+01	3
3.7E-03	3.0E-03	4.4E-03			2
6.4E-04	2.8E-04	1.0E-03			2
2.5E-03					1
4.4E-03					1
1.6E-03					1
2.4E-04	7.5E-05	3.6E-04	1.5E-04	6.2E+01	3
4.0E-04					1
9.2E-04	5.0E-05	2.9E-03	1.3E-03	1.4E+02	4
1.6E-03					1
3.5E-03					1
3.0E-04					1
3.3E-04	1.6E-04	5.0E-04			2
7.4E-04					1
3.0E-05					1

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APPENDIX I:

The following page presents an individual sample fuel mixture composition data table for Diesel (#2) fuel oil. This table, and an additional 138 tables describing the composition of the eleven petroleum fuel mixtures addressed in this document can be found on the world wide web site for the Association for the Environmental Health of Soils, www.aehs.com.

INDIVIDUAL SAMPLE FUEL MIXTURE COMPOSITION DATA

fuel mixture: **Diesel (#2) Fuel Oil**
sample #: **24/D1 Swedish Sample**
from: **Westerholm, R. and H. Li, Environmental Science & Technology, Vol 28, No. 5, pp. 965-972, 1994**

compound class	carbon #	compound	weight percent	# of data points	flag(s)
Alkenes		Total Alkenes	1.4E+00%	1	7
Inorganics		Total Sulfur	1.0E-02%	1	21
		Water	1.5E-04%	1	15
Polynuclear Aromatics		Total Triaromatics	7.0E-02%	1	7
	14	Anthracene	3.0E-06%	1	6
	14	Phenanthrene	1.9E-04%	1	6
	15	1-Methylphenanthrene	1.1E-05%	1	6
	15	2-Methylanthracene	2.0E-05%	1	6
	15	3-Methylphenanthrene	2.1E-05%	1	6
	15	4- & 9-Methylphenanthrene	1.4E-05%	1	6
	16	Fluoranthene	1.6E-05%	1	6
	16	Pyrene	1.8E-05%	1	6
	17	1-Methylpyrene	6.4E-06%	1	6
	17	2-Methylpyrene	4.8E-06%	1	6
	17	Benzo(a)fluorene	6.5E-07%	1	6
	18	1-Methyl-7-isopropylphenanthrene	1.5E-06%	1	6
	18	Benz(a)anthracene	4.0E-06%	1	6
	18	Benzo(g,h,i)fluoranthene	3.4E-07%	1	6
	18	Chrysene and Triphenylene	4.9E-06%	1	6
	20	Benzo(b+k)fluoranthene	5.8E-07%	1	6
	20	Benzo(e)pyrene	5.5E-06%	1	6
	21	Cyclopenta(cd)pyrene	6.6E-06%	1	6
	22	Benzo(g,h,i)perylene	9.1E-07%	1	6
	22	Indeno(1,2,3-cd)pyrene	6.4E-07%	1	6
	22	Picene	3.5E-07%	1	6
Total Aromatics		Total Aromatics	2.0E+00%	1	7 14
Total Cycloalkanes		Total Cycloalkanes	5.4E+01%	1	21
Total Diaromatics (Including Naphthalenes)		Total Diaromatics (Including Naphthalenes)	7.3E-02%	1	7
Total Polynuclear Aromatics		Total Polynuclear Aromatics	1.6E-04%	1	6
Total Straight-Chain and Branched Alkanes		Total Straight-Chain and Branched Alkanes	4.6E+01%	1	21

flag(s)

6 Data was converted using formula WT%=mg/L*(1/0.8762)*10-4.

7 Data was converted using formula WT%=vol%*d(analyte)/d(product), assuming d(aromatic,olefins)=0.867g/mL, d(alkanes)=0.73mg/L, d(PAHs)=1.26mg/L, d(lube oil)=0.89mg/L, d(fuel#2,

14 Assuming 30% PAHs and 70% monoaromatics.

15 Data was converted using formula WT%=ppm*10-4.

21 no flag