

ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA

ENTRY FOR 1-METHYLPHENANTHRENE

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Like a library or many large databases (such as EPA's national STORET water quality database), this document contains information of variable quality from very diverse sources. In compiling this document, mistakes were found in peer reviewed journal articles, as well as in databases with relatively elaborate quality control mechanisms [366,649,940]. A few of these were caught and marked with a "[sic]" notation, but undoubtedly others slipped through. The [sic] notation was inserted by the editors to indicate information or spelling that seemed wrong or misleading, but which was nevertheless cited verbatim rather than arbitrarily changing what the author said.

Most likely additional transcription errors and typos have been added in some of our efforts. Furthermore, with such complex subject matter, it is not always easy to determine what is correct and what is incorrect, especially with the "experts" often disagreeing. It is not uncommon in scientific research for two different researchers to come up with different results which lead them to different conclusions. In compiling the Encyclopedia, the editors did not try to resolve such conflicts, but rather simply reported it all.

It should be kept in mind that data comparability is a major problem in environmental toxicology since laboratory and field methods are constantly changing and since there are so many different "standard methods" published by EPA, other federal agencies, state agencies, and various private groups. What some laboratory and field investigators actually do for standard operating practice is often a unique combination of various standard protocols and impromptu "improvements." In fact, the interagency task force on water methods concluded that [1014]:

It is the exception rather than the rule that water-quality monitoring data from different programs or time periods can be compared on a scientifically sound basis, and that...

No nationally accepted standard definitions exist for water quality parameters. The different organizations may collect data using identical or standard methods, but identify them by different names, or use the same names for data collected by different methods [1014].

Differences in field and laboratory methods are also major issues related to (the lack of) data comparability from media other than water: soil, sediments, tissues, and air.

In spite of numerous problems and complexities, knowledge is often power in decisions related to chemical contamination. It is therefore often helpful to be aware of a broad universe of conflicting results or conflicting expert opinions rather than having a portion of this information arbitrarily censored by someone else. Frequently one wants to know of the existence of information, even if one later decides not to use it for a particular application. Many would like to see a high percentage of the information available and decide for themselves what to throw out, partly because they don't want to seem uninformed or be caught by surprise by potentially important information. They are in a better position if they can say: "I knew about that data, assessed it based on the following quality assurance criteria, and decided not to use it for this application." This is especially true for users near the end of long decision processes, such as hazardous site cleanups, lengthy ecological risk assessments, or complex natural resource damage assessments.

For some categories, the editors found no information and inserted the phrase "no information found." This does not necessarily mean that no information exists; it

simply means that during our efforts, the editors found none. For many topics, there is probably information "out there" that is not in the Encyclopedia. The more time that passes without encyclopedia updates (none are planned at the moment), the more true this statement will become. Still, the Encyclopedia is unique in that it contains broad ecotoxicology information from more sources than many other reference documents. No updates of this document are currently planned. However, it is hoped that most of the information in the encyclopedia will be useful for some time to come even without updates, just as one can still find information in the 1972 EPA Blue Book [12] that does not seem well summarized anywhere else.

Although the editors of this document have done their best in the limited time available to insure accuracy of quotes or summaries as being "what the original author said," the proposed interagency funding of a bigger project with more elaborate peer review and quality control steps never materialized.

The bottom line: The editors hope users find this document useful, but don't expect or depend on perfection herein. Neither the U.S. Government nor the National Park Service make any claims that this document is free of mistakes.

The following is one chemical topic entry (one file among 118). Before utilizing this entry, the reader is strongly encouraged to read the README file (in this subdirectory) for an introduction, an explanation of how to use this document in general, an explanation of how to search for power key section headings, an explanation of the organization of each entry, an information quality discussion, a discussion of copyright issues, and a listing of other entries (other topics) covered.

See the separate file entitled REFERENC for the identity of numbered references in brackets.

HOW TO CITE THIS DOCUMENT: As mentioned above, for critical applications it is better to obtain and cite the original publication after first verifying various data quality assurance concerns. For more routine applications, this document may be cited as:

Irwin, R.J., M. VanMouwerik, L. Stevens, M.D. Seese, and W. Basham. 1997. Environmental Contaminants Encyclopedia. National Park Service, Water Resources Division, Fort Collins, Colorado. Distributed within the Federal Government as an Electronic Document (Projected public availability

on the internet or NTIS: 1998).

Phenanthrene, 1-Methyl- (1-Methylphenanthrene, CAS number 832-69-9)

NOTE: Currently there is relatively little information available on specific alkyl homologs of phenanthrene. Thus many of the sections listed below contain the phrase "No information found." In such cases, until more information is available, the following data interpretation procedures are recommended:

To interpret concentrations of this particular grouping of alkyl polycyclic aromatic hydrocarbons (PAHs), the reader may first total phenanthrene concentrations and then compare the total to phenanthrene benchmarks. The concentration of total phenanthrenes is the sum of the following concentrations: total C1 phenanthrenes (including all methyl phenanthrenes) + total C2 phenanthrenes (including dimethylphenanthrenes) + total C3 phenanthrenes (including trimethyl phenanthrenes) + total C4 phenanthrenes + C0 (phenanthrene parent compound concentration). Such tentative comparisons are justified on the basis that alkyl PAHs often (there may be exceptions) tend to be equally or more toxic, be equally phototoxic, and be equally or more carcinogenic than the parent compound PAH (see "PAHs as a group" entry).

In the case of text discussion sections where little or no information is available on this particular grouping alkyl PAHs, the reader is encouraged to also read the "parent" entries (in this case, the phenanthrene), but to keep in mind the generalizations (there may be exceptions) that alkyl PAHs often tend to be more persistent, have higher KOWs, be less volatile, be less soluble, be less mobile, bioaccumulate more, have different chemical/physical characteristics, be equally or more toxic, be equally phototoxic, and be equally or more carcinogenic than the parent compound PAH.

Brief Introduction:

Br.Class: General Introduction and Classification Information:

1-Methylphenanthrene is an alkylated phenanthrene; phenanthrene is a low molecular weight, three-ring polyaromatic hydrocarbon (PAH) [697].

1-Methylphenanthrene is present as a major component of the total content of PAHs in the environment [847]. Human exposure to 1-methylphenanthrene occurs primarily through the smoking of tobacco, inhalation of polluted air, and by ingestion of food and water contaminated by combustion effluents [847].

1-Methylphenanthrene is a C1 alkyl homolog of phenanthrene, often (though not always) analyzed for by a GC/MS/SIM expanded scan for PAHs and alkyl PAHs (such as the NOAA Protocol expanded scan) [828,697].

1-Methylphenanthrene is included in C1-phenanthrene/ reported concentrations. This reported value includes all phenanthrenes that have one carbon group attached. (C1-phenanthrene and C1- compounds cannot be differentiated with current (1996) analytical techniques.) The concentration of just 1-methylphenanthrene is also often reported on expanded PAH scan lists [828].

Br.Haz: General Hazard/Toxicity Summary:

Studies conclude that the toxicity of an oil appears to be a function of its di-aromatic and tri-aromatic hydrocarbons, which includes three-ring hydrocarbons such as phenanthrene [770].

The heavier (4-, 5-, and 6-ring) PAHs are more persistent than the lighter 3-ring PAHs such as all C1-phenanthrenes and tend to have greater carcinogenic and other chronic impact potential [796].

Probably the most important target analytes in natural resource damage assessments for oil spills are PAHs and the homologous series (alkylated) PAHs [468]. Alkylated PAHs are more abundant, persist for a longer time, and are sometimes more toxic than the parent PAHs [468]. Alkyl substitution usually decreases water solubility [754]. They also tend to bioaccumulate to a greater degree [347,885].

Within an aromatic series, acute toxicity increases with increasing alkyl substitution on the aromatic nucleus [851]. For example, there is an increase in toxicity as alkylation of the naphthalene structure increases. The order of most toxic to least in a study using grass shrimp (*Palaemonetes pugio*) and brown shrimp (*Penaeus aztecus*) was dimethylnaphthalenes (C2-) > methylnaphthalenes (C1-) > naphthalenes [853]. Since alkyl PAHs are often more abundant in fresh petroleum products than their parent compounds, and the proportion of alkyl PAHs to parent compound PAHs increases as the oil ages, it is very important to analyze oil samples for alkyl PAHs any time that biological effects are a concern.

Although there is less toxicity information available for most of the alkyl PAHs than for their parent compounds, most alkyl PAHs appear to be at least as toxic or

hazardous as the parent compound. Thus, for now, risk assessment experts suggest interpreting alkyl homolog values against known toxicological effects benchmarks and criteria for the respective parent compound (Bill Stubblefield, ENSR, personal communication, 1995).

Acute toxicity is rarely reported in humans, fish, or wildlife, as a result of exposure to low levels of a single PAH compound such as this one. PAHs in general are more frequently associated with chronic risks. These risks include cancer and often are the result of exposures to complex mixtures of chronic-risk aromatics (such as PAHs, alkyl PAHs, benzenes, and alkyl benzenes), rather than exposures to low levels of a single compound (Roy Irwin, National Park Service, Personal Communication, 1996, based on an overview of literature on hand). See also "PAHs as a group" entry.

This alkyl PAH often occur together with other aromatics (sometimes including alkyl PAHs), and a typical complex mixture of aromatics may be more toxic or hazardous in general than this particular group of alkyl PAHs would be alone (see "PAHs as a group" entry). Anthracene is one of the more phototoxic PAHs (See also: entries for anthracene and phenanthrene).

Br.Car: Brief Summary of Carcinogenicity/Cancer Information:

Little information found on this alkyl PAH. See also entry for Phenanthrene.

The available data are inadequate to permit an evaluation of the carcinogenicity of 1-methylphenanthrene to experimental animals [847]. Also, the International Agency for Research on Cancer (IARC) and the EPA have determined that phenanthrene is not classifiable as to its carcinogenicity to humans [788,847].

However, alkyl substitution often confers or enhances carcinogenic potential of PAHs. A few examples:

Very few alkyl PAHs have been broadly tested for carcinogenicity, but it is known that both dimethylbenzo(a)anthracene and its parent compound benzo(a)anthracene are carcinogenic [40,793,788,881]. Methylbenzo(a)anthracene is actually more carcinogenic than its parent compound benzo(a)anthracene, and dimethylbenzo(a)anthracene is still more carcinogenic [40].

Both cholanthrene and its 3 methyl alkyl cholanthrene counterpart are carcinogenic [40,793]. It is also known that alkylation does not

significantly change phototoxicity [888] and that there are some relationships between phototoxicity and potential carcinogenicity (see discussion above). Thus it would not be surprising to discover that a notable number of alkyl PAHs are carcinogenic although they are not now typically added to the list of "carcinogenic PAHs" considered in risk assessments.

This alkyl PAH often occurs together with other PAHs, in complex mixtures possibly more carcinogenic than the individual components (see "PAHs as a group" entry). The debates on exactly how to perform both ecological and human risk assessments on the complex mixtures of PAHs typically found at contaminated sites, are likely to continue. There are some clearly wrong ways to go about it, but defining clearly right ways is more difficult. PAHs such as these usually occur in complex mixtures rather than alone. One of the few things that seems clear is that complex PAH mixtures in water, sediments, and organism internal tissues may be carcinogenic and/or phototoxic (Roy Irwin, National Park Service, personal communication, 1996; see also "PAHs as a group" entry and Arfsten et al [911]).

One way to approach site specific risk assessments is to collect the complex mixture of PAHs and other lipophilic organic contaminants in a semipermeable membrane device (SPMD, also known as a fat bag) [894,895,896], retrieve the organic contaminant mixture from the SPMD, then test the mixture for carcinogenicity, toxicity, and phototoxicity (James Huckins, National Biological Service, and Roy Irwin, National Park Service, personal communication, 1996).

Information from RTECS [607]:

IARC Cancer Review:Animal Inadequate Evidence
REFERENCE: IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man 32:405, 1983.
IARC Cancer Review:Human No Adequate Data
REFERENCE: IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man 32:405, 1983.

IARC Cancer Review:Group 3 REFERENCE: IARC Monographs, Supplement 7:56, 1987.

Since there is little information concerning carcinogenicity of this group of alkyl PAH compounds, the following information about the parent compound phenanthrene is provided:

EPA 1996 IRIS database information [893]:

Evidence for classification as to human carcinogenicity; weight-of-evidence classification:

Classification: D; not classifiable as to human carcinogenicity

BASIS: Based on no human data and inadequate data from a single gavage study in rats and skin painting and injection studies in mice.

HUMAN CARCINOGENICITY DATA: None.

ANIMAL CARCINOGENICITY DATA: Inadequate.

EPA Historical (modeling purposes only)
Classification: Carcinogen [302,446].

Several references [887,888,891] do not include phenanthrene among PAHs found to be phototoxic, but one reference does list it as phototoxic [494]. Although not definitive, as discussed above, phototoxicity represents one clue suggesting possible carcinogenicity.

Br.Dev: Brief Summary of Developmental, Reproductive, Endocrine, and Genotoxicity Information:

No information found. See Phenanthrene entry.

Br.Fate: Brief Summary of Key Bioconcentration, Fate, Transport, Persistence, Pathway, and Chemical/Physical Information:

The heavier (4-, 5-, and 6-ring) PAHs are more persistent than the lighter 3-ring PAHs such as all C1-phenanthrenes [796].

Introduction or extension of an alkyl group increases persistence and lipophilicity; increased lipophilicity is often associated with increased absorption [856].

Low molecular weight PAHs (naphthalenes through phenanthrenes) are removed from the water column primarily by evaporation, microbial oxidation, and sedimentation [851].

Partitioning of phenanthrene to sediment is generally expected whenever phenanthrene is released to water [336].

Two significant processes which can influence the fate of

phenanthrene in the sediment are sorption and biodegradation. Oxidation, hydrolysis and volatilization processes were found to have no effect on the fate of phenanthrene in sediment [862].

Synonyms/Substance Identification:

1-Methylphenanthrene [847]
Phenanthrene, 1-Methyl- [847]

Molecular formula [848]:
C15-H12

Associated Chemicals or Topics (Includes Transformation Products):

See also individual entries:

Phenanthrene
Phenanthrene/Anthracene, C1-
PAHs, Alkyl Homologs of
PAHs as a group
Petroleum, General

Water Data Interpretation, Concentrations and Toxicity (All Water Data Subsections Start with "W."):

W.Low (Water Concentrations Considered Low):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.High (Water Concentrations Considered High):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.Typical (Water Concentrations Considered Typical):

Tap water [847]: 1-Methylphenanthrene was found in tap water at a concentration of 0.37 ug/L.

W.Concern Levels, Water Quality Criteria, LC50 Values, Water Quality Standards, Screening Levels, Dose/Response Data, and Other Water Benchmarks:

W.General (General Water Quality Standards, Criteria, and Benchmarks Related to Protection of Aquatic Biota in General; Includes Water Concentrations Versus Mixed or General Aquatic Biota):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.Plants (Water Concentrations vs. Plants):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.Invertebrates (Water Concentrations vs. Invertebrates):

LC50 Values [851]:

Neanthes arenaceodentata
(marine polychaete) - 0.3 ppm, 96 h

W.Fish (Water Concentrations vs. Fish):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.Wildlife (Water Concentrations vs. Wildlife or Domestic Animals):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.Human (Drinking Water and Other Human Concern Levels):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

W.Misc. (Other Non-concentration Water Information):

Several references [887,888,891] do not include phenanthrene among PAHs found to be phototoxic, but one reference does list it as phototoxic [494].

Sediment Data Interpretation, Concentrations and Toxicity (All Sediment Data Subsections Start with "Sed."):

Sed.Low (Sediment Concentrations Considered Low):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.High (Sediment Concentrations Considered High):

1-Methylphenanthrene was detected in 95.3 percent of urban-bay sample from the Puget Sound area. The mean concentration was 645.97 ug/kg dry weight (ppb), while the median concentration was 68 ug/kg (ppb) [852].

NOTE: The above values are not normalized for total organic carbon (TOC) content.

Sed.Typical (Sediment Concentrations Considered Typical):

1-Methylphenanthrene was detected in 60 percent of non-urban-bay samples from the Puget Sound area. The mean concentration was 91.4 ug/kg dry weight (ppb), while the median concentration was 8.1 ug/kg (ppb) [852].

NOTE: The above values are not normalized for total organic carbon (TOC) content.

Sed.Concern Levels, Sediment Quality Criteria, LC50 Values, Sediment Quality Standards, Screening Levels, Dose/Response Data and Other Sediment Benchmarks:

Sed.General (General Sediment Quality Standards, Criteria, and Benchmarks Related to Protection of Aquatic Biota in General; Includes Sediment Concentrations Versus Mixed or General Aquatic Biota):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.Plants (Sediment Concentrations vs. Plants):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.Invertebrates (Sediment Concentrations vs. Invertebrates):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.Fish (Sediment Concentrations vs. Fish):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.Wildlife (Sediment Concentrations vs. Wildlife or Domestic Animals):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.Human (Sediment Concentrations vs. Human):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Sed.Misc. (Other Non-concentration Sediment Information):

No information found.

Soil Data Interpretation, Concentrations and Toxicity (All Soil Data Subsections Start with "Soil."):

Soil.Low (Soil Concentrations Considered Low):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.High (Soil Concentrations Considered High):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Typical (Soil Concentrations Considered Typical):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Concern Levels, Soil Quality Criteria, LC50 Values, Soil Quality Standards, Screening Levels, Dose/Response Data and Other Soil Benchmarks:

Soil.General (General Soil Quality Standards, Criteria, and Benchmarks Related to Protection of Soil-dwelling Biota in General; Includes Soil Concentrations Versus Mixed or General Soil-dwelling Biota):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Plants (Soil Concentrations vs. Plants):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Invertebrates (Soil Concentrations vs. Invertebrates):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Wildlife (Soil Concentrations vs. Wildlife or Domestic Animals):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Human (Soil Concentrations vs. Human):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Soil.Misc. (Other Non-concentration Soil Information):

No information found.

Tissue and Food Concentrations (All Tissue Data Interpretation Subsections Start with "Tis."):

Tis.Plants:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Plants:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

B) Body Burden Residues in Plants: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Tis.Invertebrates:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Invertebrates:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

B) Concentrations or Doses of Concern in Food Items Eaten by Invertebrates:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

C) Body Burden Residues in Invertebrates: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

Details of phenanthrene content (ug/kg or ppb) in whole body samples of mussels) from Snug Harbor, Alaska, an area heavily oiled by the Exxon Valdez Crude Oil, 4/15/89 [971]:

Note: Concurrent measurements of water quality, as well as equilibrium partitioning estimates of water quality based on concentrations in fish and mussels, both confirm that PAH concentrations did not exceed water quality criteria at the time these concentrations were measured in mussel tissues [971]. These values are wet weight (Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996):

phenanthrene: 356 ug/kg = ppb

C1-phenanthrene: 1924 ug/kg = ppb
C2-phenanthrene: 3834 ug/kg = ppb
C3-phenanthrene: 2438 ug/kg = ppb
C4-phenanthrene: 796 ug/kg = ppb

Tis.Fish:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Fish (Includes FDA Action Levels for Fish and Similar Benchmark Levels From Other Countries):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

B) Concentrations or Doses of Concern in Food Items Eaten by Fish:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

C) Body Burden Residues in Fish: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

Details of phenanthrene content (mg/kg or ppm) in salmon carcass (fatty viscera removed, so the concentrations may have been higher from whole body samples) from Snug Harbor, Alaska, an area heavily oiled by the Exxon Valdez Crude Oil, 4/15/89 [971]:

Note: Concurrent measurements of water quality, as well as equilibrium partitioning estimates of water quality based on concentrations in fish and mussels, both confirm that PAH concentrations did not exceed water quality criteria at the time these concentrations were measured in fish tissues [971]. These values are wet weight (Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996):

phenanthrene: 22.97 ug/kg = ppb
C1-phenanthrene: 28.48 ug/kg = ppb
C2-phenanthrene: 20.45 ug/kg = ppb
C3-phenanthrene: 12.43 ug/kg = ppb
C4-phenanthrene: 1.71 ug/kg = ppb

Tis.Wildlife: Terrestrial and Aquatic Wildlife, Domestic Animals and all Birds Whether Aquatic or not:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Wildlife, Domestic Animals, or Birds:

No information found. Compare total phenanthrenes

to phenanthrene benchmarks.

B) Concentrations or Doses of Concern in Food Items Eaten by Wildlife, Birds, or Domestic Animals (Includes LD50 Values Which do not Fit Well into Other Categories, Includes Oral Doses Administered in Laboratory Experiments):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

C) Body Burden Residues in Wildlife, Birds, or Domestic Animals: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

B) Concentrations or Doses of Concern in Food Items Eaten by Humans (Includes Allowable Tolerances in Human Food, FDA, State and Standards of Other Countries):

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

C) Body Burden Residues in Humans: Typical, Elevated, or of Concern Related to the Well-being of Humans:

No information found. Compare total phenanthrenes to phenanthrene benchmarks.

Tis.Misc. (Other Tissue Information):

Several references [887,888,891] do not include phenanthrene among PAHs found to be phototoxic, but one reference does list it as phototoxic [494].

Bio.Detail: Detailed Information on Bioconcentration, Biomagnification, or Bioavailability:

During the Exxon Valdez spill, bioconcentration explained the buildup of PAHs in tissues better than biomagnification; most accumulation was of an equilibrium partitioning nature across the gills rather than from the food chain [971]. Immature fish seem to have higher bioconcentration of PAHs than adults, perhaps because their PAH breakdown systems are not fully developed and at times

perhaps because of a higher percentage of lipid tissues (yolk tissues, etc) [971] (confirmed by Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996).

Alkyl PAHs tend to bioaccumulate to a greater degree than parent compound PAHs [347,885]. Introduction or extension of an alkyl group increases lipophilicity, which often appears as increased absorption [856].

Interactions:

No information found.

Uses/Sources:

See Chem.Detail section below for 1-methylphenanthrene concentrations in various petroleum products.

1-Methylphenanthrene occurs ubiquitously in products of incomplete combustion; it also occurs in fossil fuels. It has been identified in mainstream cigarette smoke (3.2 ug/100 cigarettes) and marijuana smoke (4.2 ug/100 cigarettes), and gasoline engine exhaust (256-404 ug/L burned fuel) [847].

Forms/Preparations/Formulations:

No information found.

Chem.Detail: Detailed Information on Chemical/Physical Properties:

Alkylation of PAHs tends to increase Kow and significantly or drastically change other physical/chemical parameters (for more detailed discussions, see Chem.detail section of "PAHs as a group" entry).

Solubility [847]: Virtually insoluble in water (269 ug/L);
soluble in ethanol

Solubility in water [848]: 0.255 - 0.27 (mg/L at 25 degrees C)

Boiling Point [848]: 359 to 390 degrees C

Melting point [847]: 123 degrees C

Molecular weight [847]: 192.3

Octanol/Water partition coefficient (low Kow) [848,849]: 5.14

Log Kow values for phenanthrenes [971]:

phenanthrene:	4.57
C1-phenanthrene:	5.14
C2-phenanthrene:	5.51
C3-phenanthrene:	6

C4-phenanthrene: 6.51

Concentrations of 1-Methylphenanthrene in South Louisiana crude, Kuwait crude, No. 2 fuel oil, and Bunker C residual were 111, --, 173, and 43 mg/kg (ppm), respectively [177].

For comparison, the following table lists some of the specific naphthalene contents (ppm) of water soluble fraction (WSF) from 10% oil-in-water solution of four test oils (measured by gas chromatography) [770]:

COMPOUNDS	SOUTH LA CRUDE	KUWAIT CRUDE	NO. 2 FUEL OIL	BUNKER C RESIDUAL
Phenanthrene	0.001	0.001	0.010	0.009
Methylphenanthrenes	0.002	0.001	0.007	0.011

Aromatic hydrocarbons concentrations (ug/g, ppb) measured in a study using Prudhoe Bay Crude oil [854]:

COMPOUNDS	CONCENTRATION (ppb)
Phenanthrene	431
1-Methylphenanthrene	221

For comparison, capillary gas chromatograph analyses of aromatic hydrocarbon concentrations (uL/L, ppb) in the water soluble fractions (WSF) of a fresh Prudhoe Bay Crude oil [854]:

COMPOUNDS	CONCENTRATION (ppb)
Phenanthrene	1.18
Methylphenanthrene	<0.08

Details of phenanthrene content (mg/kg or ppm) in one fresh sample of Exxon Valdez Crude Oil [971]:

Phenanthrene:	262 mg/kg = ppm
C1-Phenanthrene:	572 mg/kg = ppm
C2-Phenanthrene:	722 mg/kg = ppm
C3-Phenanthrene:	576 mg/kg = ppm
C4-Phenanthrene:	446 mg/kg = ppm

Fate.Detail: Detailed Information on Fate, Transport, Persistence, and/or Pathways:

Fate characteristics would be expected to be different than the parent compound in the following ways: alkyl PAHs are more persistent than the parent PAHs [468]. They also tend to bioaccumulate to a greater degree [347,885]. Alkyl substitution usually decreases water solubility [754]. See entry for parent compound.

No other information found. See entry for Phenanthrene.

Laboratory and/or Field Analyses:

Many methods have been used to analyze for PAHs [861]. For risk assessment or drinking water purposes, low detection limits should be specified using Selective Ion Mode (SIM) methods [828] or other rigorous methods.

When potential biological effects are being considered, many of the methods historically used have been determined to be inferior to the NOAA protocol expanded scan [828] being recommended by some risk assessment experts in 1996. Most of the historically used methods, including EPA standard semi-volatile scan number 8270, do not cover important alkyl PAHs and do not utilize low-enough detection limits (10 ppt for water, 0.3 to 1 ppb for tissues, sediments, and soil) to use in ecological risk assessments.

Note: Utilizing up to date techniques, many of the better labs can use detection limits of 0.3 to 1 ppb for tissues, sediments, and soils, and these lower detection limits are far better for risk or hazard assessment, but in all cases detection limits for these media should not be above 10 ppb.

Recent (1991) studies have indicated that EPA approved methods used for oil spill assessments (including total petroleum hydrocarbons method 418.1, semivolatile priority pollutant organics methods 625 and 8270, and volatile organic priority pollutant methods 602, 1624, and 8240) are all inadequate for generating scientifically defensible information for Natural Resource Damage Assessments [468]. These general organic chemical methods are deficient in chemical selectivity (types of constituents analyzed) and sensitivity (detection limits); the deficiencies in these two areas lead to an inability to interpret the environmental significance of the data in a scientifically defensible manner [468].

If a Park Service groundwater investigation at Colonial National Historical Park performed in response to contamination by Fuel Oil 5 had utilized EPA semi-volatile scan 8270 or any of the other typical EPA scans (625, etc.) all of which only include parent compounds and typically utilize detection limits in the 170-600 ppb range, the false conclusion reached would have been that no PAHs were present in significant (detection limit) amounts. This false negative conclusion would have been made because the parent compound PAHs present constituted only 7.6% of the PAHs detected in groundwater by the expanded scan [828], and the highest concentration found for any parent compound was 8.4 ppb, far below the detection limits used on the older standard EPA scans. Utilizing the NOAA protocol expanded scan [828], it was determined that 92.4% of the total concentration values of the PAHs detected in groundwater were alkyl PAHs, and that all 39 PAHs and alkyl PAHs were present. Of course, all 39 PAHs were also present in the fresh product, in much higher concentrations, and also having alkyl compounds with the highest percentage of higher values compared to parent compounds (see Chem.Detail section in separate "PAHs as a group" entry for more details).

In a similar vein, if the Park Service sediment investigation at Petersburg National Historical Battlefield (see Chem.Detail

section in separate "PAHs as a group" entry; this study was performed in response to contamination by Diesel) had utilized EPA semi-volatile scan 8270 or any of the other typical EPA scans (625, etc.), all of which only include parent compounds and often utilize detection limits no lower than the 170-600 ppb range, the false conclusion reached would have been that only one PAH was present in significant (detection limit) amounts. This false negative conclusion would have been made because the parent compound PAHs present constituted only 2.4% of the PAHs detected in sediments, and the highest concentration found for any parent compound except pyrene was 85.5 ppb, far below the detection limits used on the older standard EPA scans. Pyrene was 185 ppb, which would have been non-detected on many of the EPA scans, but not all. However, utilizing the NOAA protocol expanded scan [828], it was determined that 97.6% of total quantity of PAHs detected in sediments were alkyl PAHs, and that all 39 PAHs and alkyl PAHs were present in these sediments.

Contaminants data from different labs, different states, and different agencies, collected by different people, are often not very comparable (see also, discussion in the disclaimer section at the top of this entry).

As of 1997, the problem of lack of data comparability (not only for water methods but also for soil, sediment, and tissue methods) between different "standard methods" recommended by different agencies seemed to be getting worse, if anything, rather than better. The trend in quality assurance seemed to be for various agencies, including the EPA and others, to insist on quality assurance plans for each project. In addition to quality control steps (blanks, duplicates, spikes, etc.), these quality assurance plans call for a step of insuring data comparability [1015,1017]. However, the data comparability step is often not given sufficient consideration. The tendency of agency guidance (such as EPA SW-846 methods and some other new EPA methods for bio-concentratable substances) to allow more and more flexibility to select options at various points along the way, makes it harder to insure data comparability or method validity. Even volunteer monitoring programs are now strongly encouraged to develop and use quality assurance project plans [1015,1017].

At minimum, before using contaminants data from diverse sources, one should determine that field collection methods, detection limits, and lab quality control techniques were acceptable and comparable. The goal is that the analysis in the concentration range of the comparison benchmark concentration should be very precise and accurate.

It should be kept in mind that quality control field and lab blanks and duplicates will not help in the data quality assurance goal as well as intended if one is using a method prone to false negatives. Methods may be prone to false negatives due to the use of detection limits that are too high, the loss of contaminants through inappropriate handling, or the use of inappropriate methods. The use of inappropriate methods is particularly common related to oil products.

Less rigorous scanning methods for various PAHs in drinking water have included High pressure liquid chromatography (EPA 550,

550.1); gas chromatographic/mass spectrometry (EPA 525): PQL=
0.0002 mg/L [893].