

ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA
ENTRY FOR C1-PHENANTHRENES + C1 ANTHRACENES

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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/anthracene, C1- (C1-Phenanthrenes + C1 Anthracenes)

NOTE: Currently there is relatively little information available on specific alkyl homologs of combined phenanthrenes and anthracenes. 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 PAHs, the reader may first total phenanthrene and anthracene concentrations and then compare the total to phenanthrene and/or anthracene benchmarks. The concentration of total phenanthrenes and anthracenes is the sum of the following concentrations: total C1 phenanthrenes and anthracenes (including all methyl phenanthrenes and anthracenes) + total C2 phenanthrenes and anthracenes (including dimethylphenanthrenes and anthracenes) + total C3 phenanthrenes and anthracenes (including trimethyl phenanthrenes and anthracenes) + total C4 phenanthrenes and anthracenes + C0 (phenanthrene and anthracene 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 of alkyl PAHs, the reader is encouraged to also read the "parent" entries (in this case, the phenanthrene and the anthracene entries), 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:

The phrase C1-phenanthrene/anthracene refers to a group of alkyl phenanthrene and anthracene compounds which all have one carbon group (that is, one methyl group) attached. Both phenanthrene and anthracene are three-ring PAHs, so all the C1-phenanthrene/anthracenes are three-ring PAHs with one methyl group attached. C1-

phenanthrene and C1-anthracene compounds cannot be differentiated with current (1996) analytical techniques. C1-phenanthrene/anthracenes differ from the parent compounds phenanthrene and anthracene in that there is one carbon group attached to C1-phenanthrene/anthracenes while there are none attached to phenanthrene or anthracene. C1-phenanthrene/anthracenes differ from C2-phenanthrene/anthracenes in that there is one rather than two carbon groups attached. C1-phenanthrene/anthracene is a naming convention for reporting the total of all detected C1 alkyl homologs of phenanthrene and anthracene.

C1-phenanthrene/anthracenes is included on the expanded scan of PAHs and alkyl PAHs recommended by NOAA [828]; this list includes the PAHs recommended by the NOAA's National Status and Trends program [680].

C1-phenanthrene/anthracene reported concentrations represent the total concentration of all C1 phenanthrenes and C1 anthracenes. Some common examples of C1-phenanthrene/anthracenes include (Tom McDonald, Texas A&M, personal communication, 1995):

- 9-Methylphenanthrene
- 3-Methylphenanthrene
- 2-Methylphenanthrene
- 1-Methylphenanthrene
- 2-Methylanthracene
- 9-Methylanthracene

Br.Haz: General Hazard/Toxicity Summary:

Probably the most important target analytes in natural resource damage assessments for oil spill 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]. 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 adding (lumping) all alkyl homolog concentrations with its constituent parent

concentration, and interpreting that grouped value (Bill Stubblefield, ENSR, Fort Collins, Personal Communication, 1995). For example, add the reported concentrations for C1-, C2-, C3-, and C4-phenanthrene/anthracenes to the reported phenanthrene/anthracene concentration, and interpret that total value against known toxicological effects benchmarks or criteria for phenanthrene and anthracene.

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

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.

These alkyl PAHs 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:

No information found on this group of alkyl PAHs. See entries for anthracene and phenanthrene.

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 group of alkyl PAHs often occurs together with other PAHs, some of which may be more carcinogenic. The debates on which PAHs and alkyl PAHs to classify as carcinogens, and the details of 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. One of the few things that is clear is that PAH mixtures in water, sediments, and organism internal tissues tend to be carcinogenic and phototoxic [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).

Since there is little information concerning carcinogenicity of this group of alkyl PAH compounds, the following information about anthracene, one of the more phototoxic parent compounds related to this group of alkyl PAHs, is provided:

IRIS 1996 information from EPA on anthracene parent compound [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 animal bioassays.

HUMAN CARCINOGENICITY DATA: None.

ANIMAL CARCINOGENICITY DATA: Inadequate.

The International Agency for Research on Cancer (IARC) and recent (1994) EPA weight-of-evidence evaluations have determined that anthracene is not classifiable as to its carcinogenicity to humans [788,881].

Anthracene has not been treated as carcinogen for model calculation purposes in some EPA risk-based (RBC and PRG) models [868,903], but this tentative distinction was made for the purpose of choosing a modeling scenario based on current (often inadequate) knowledge rather than for the purpose of strongly stating that anthracene is definitely not a carcinogen; the non-carcinogenic benchmarks are sometimes nearly as low as the carcinogenic benchmarks (Stan Smucker, personal communication, EPA, 1996).

A significant increase in the formation of non-neoplastic melanotic tumors was observed among first and second generation progeny of *Drosophila melanogaster* that had been exposed chronically as larvae to low concentrations of anthracene. It was concluded that anthracene solubilized with detergents could induce autosomal dominant melanotic tumors [366, Corwin HD, Gottlieb FJ; Environ Res 15: 327-31 (1978) as cited in ITC/USEPA; Information Review #227 (Draft) Anthracene p.227 (1981)].

Anthracene is a very phototoxic PAH [887]. Phototoxic [494,911]. Although not definitive, as discussed above, phototoxicity represents one clue suggesting possible carcinogenicity. UV light greatly increases the toxicity of anthracene to bluegill sunfish [841].

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

No information found. See entries for anthracene and phenanthrene.

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 or anthracenes [796].

These compounds are alkyl PAHs, so the following generalizations concerning alkyl vs. parent compound PAHs should be kept in mind:

Some alkyl PAHs tend to be less volatile than parent compound PAHs [867]. Alkyl substitution usually also decreases water solubility [754].

Introduction or extension of an alkyl group increases not only persistence but also lipophilicity; increased lipophilicity is often associated with increased absorption [856]. Alkyl PAHs tend to bioaccumulate to a greater degree than parent compound PAHs [347,885].

Alkylated PAHs are often more abundant than parent compounds [468], at least those alkyl PAHs originating from petrogenic sources [942]. For several PAH families (naphthalenes, fluorenes, phenanthrenes, dibenzothiophenes, and chrysenes) if the unsubstituted parent PAH is less abundant than the sum of its counterpart alkyl homologues, the source is more likely petrogenic (from crude oil or other petroleum sources) rather than pyrogenic (from high temperature sources) [942].

Alkyl PAHs also tend to persist for a longer time than the parent PAHs [468, 856]. PAH persistence tends to increase with increasing alkyl substitution; for example, methyl naphthalene is more persistent than naphthalene (the parent compound) and dimethyl naphthalene is still more persistent than methyl naphthalene in sediments and amphipod tissues [885].

Comparing PAHs and alkyl PAHs, the parent compound is typically the first to degrade. Thus, as mixed composition petroleum products age, the percentage of alkyl PAHs vs. PAHs increases, yet most standard EPA scans (even 8270) do not pick up alkyl PAHs [796]. This, coupled with the need for lower detection limits and the general hazards presented by alkyl PAHs, is one reason the NOAA protocol expanded scan [828] or other rigorous scans using Selected Ion Monitoring (SIM) [942] are often recommended rather than the older standard EPA scans.

See also: entries for anthracene and phenanthrene.

Synonyms/Substance Identification:

No information found.

Associated Chemicals or Topics (Includes Transformation Products):

See also individual entries:

Anthracene
Phenanthrene
Phenanthrene, 1-Methyl
PAHs as a group
PAH, Alkyl Homologs of
Phenanthrenes/Anthracenes, C2-
Phenanthrenes/Anthracenes, C3-
Phenanthrenes/Anthracenes, C4-

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

W.Low (Water Concentrations Considered Low):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

W.High (Water Concentrations Considered High):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

W.Typical (Water Concentrations Considered Typical):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

Cautionary note: Anthracene is a very phototoxic compound [494,887,911] (see more detailed discussion of phototoxicity in the "PAHs as a group" entry). Therefore, any of the water criteria which have been developed for it using bioassays performed in the absence of UV light may be under-protective. Phototoxicity of certain PAHs was discovered when organisms which had survived lab exposures to PAHs died quickly after being moved into sunlight. An increase in toxicity due

to photo-induced changes is called phototoxicity. For certain PAHs, tests performed in the presence of UV or other solar radiation show greatly increased toxicity to those same organisms at PAH concentrations below maximum solubility [887,888,889,911].

W.Plants (Water Concentrations vs. Plants):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

W.Invertebrates (Water Concentrations vs. Invertebrates):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

W.Fish (Water Concentrations vs. Fish):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

Caution: anthracene is a very phototoxic PAH [887]. Phototoxic [494,911]. UV light greatly increases the toxicity of anthracene to bluegill sunfish [841].

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

Sed.Low (Sediment Concentrations Considered Low):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Sed.High (Sediment Concentrations Considered High):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Sed.Typical (Sediment Concentrations Considered Typical):

2-methylphenanthrene was detected in 100 % of urban-bay samples from the Puget Sound area. The mean concentration was 822 ug/kg dry weight (ppb), while the median concentration was 84.5 ug/kg (ppb) [852].

2-methylphenanthrene was detected in 100 % of non-urban-bay samples from the Puget Sound area. The mean concentration was 70 ug/kg dry weight (ppb), while the median concentration was 6 ug/kg (ppb) [852]. Note that mean and median values based on only three samples.

3-methylphenanthrene was detected in 100 % of urban-bay samples from the Puget Sound area. The mean concentration was 1613 ug/kg dry weight (ppb), while the median concentration was 61 ug/kg (ppb) [852].

3-methylphenanthrene was detected in 100 % of non-urban-bay samples from the Puget Sound area. The mean concentration was 390 ug/kg dry weight (ppb), while the median concentration was 390 ug/kg (ppb) [852]. Note that mean and median values based on only one sample.

NOTE: The above values from [852] are not normalized for total organic carbon (TOC) content. Some urban bay concentrations may be lower than non-urban bay concentrations due to more frequent dredging practices in urban bays, and also to the fact that most of the urban bays are at the mouths of rivers which are continually depositing "clean" sediment into these bays.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

Sed.Plants (Sediment Concentrations vs. Plants):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Sed.Invertebrates (Sediment Concentrations vs. Invertebrates):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Sed.Fish (Sediment Concentrations vs. Fish):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Sed.Human (Sediment Concentrations vs. Human):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

Caution: anthracene is a very phototoxic PAH [887]. Phototoxic [494,911]. UV light greatly increases the toxicity of anthracene to bluegill sunfish [841].

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

Soil.Low (Soil Concentrations Considered Low):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Soil.High (Soil Concentrations Considered High):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Soil.Typical (Soil Concentrations Considered Typical):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

Soil.Plants (Soil Concentrations vs. Plants):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Soil.Invertebrates (Soil Concentrations vs. Invertebrates):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Soil.Human (Soil Concentrations vs. Human):

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See entries for anthracene and phenanthrene.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Tis.Invertebrates:

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

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. See Br.Fate section above as well as phenanthrene and anthracene entries.

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

No information found. See Br.Fate section above as well as phenanthrene and anthracene entries.

Tis.Misc. (Other Tissue Information).

Caution: anthracene is a very phototoxic PAH [887]. Phototoxic [494,911]. UV light greatly increases the toxicity of anthracene to bluegill sunfish [841]..

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 typically bioconcentrate to a greater degree and degrade more slowly than their parent compounds (see phenanthrene and anthracene entries for information on the parent compound). Introduction or extension of an alkyl group increases lipophilicity, which often appears as increased absorption. No other information found. See entries for anthracene and phenanthrene.

Interactions:

No information found. See entries for anthracene and phenanthrene.

Uses/Sources:

See Chem.Detail section below for C1-phenanthrene/anthracene concentrations in various petroleum products.

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).

Log Kow values for phenanthrenes [971]:

phenanthrene:	4.57
C1-phenanthrene:	5.14
C2-phenanthrene:	5.51
C3-phenanthrene:	6
C4-phenanthrene:	6.51

The following information is for 1-methylphenanthrene only, just one of the compounds in this group of alkyl PAHs (CAS number 832-69-6):

Water Solubility [848]: 0.255 to 0.27 mg/L at 25 degrees C
Boiling Point [848]: 359 to 390 degrees C
Melting Point [848]: 119 to 123 degrees C
Octanol/Water Partition Coefficient, log Kow [848]: 5.14

The following information is for 2-methylanthracene (CAS number 613-12-7):

Water Solubility [848]: 0.023 to 0.281 mg/L at 25 degrees C
(most values 0.027 to 0.039 mg/L)
Boiling Point [848]: 359 degrees C
Melting Point [848]: 199 to 209 degrees C
Octanol/Water Partition Coefficient, log Kow [848]: 5.15

The following information is for 9-methylanthracene (CAS number 779-02-2):

Water Solubility [848]: 0.206 to 0.801 mg/L at 25 degrees C
(most values 0.257 to 0.269 mg/L)
Boiling Point [848]: 345 degrees C
Melting Point [848]: 80 to 82 degrees C
Octanol/Water Partition Coefficient, log Kow [848]: 4.61 to 5.61 (most values 5.07 to 5.12)

C1-phenanthrenes/anthracenes concentrations were determined for three different crude oil sample types taken from the Exxon Valdez oil spill. Concentrations in 1) unweathered oil from the tanker itself (March 1989), 2) oil skimmed from the water immediately after the spill and held in the skimmer barge for about 90 days (July 1989), and 3) weathered oil from Prince William Sound

shorelines (May 1989) were: 488, 660, and 410 ug/g oil sampled, respectively [790; Reprinted with permission from Environmental Toxicology and Chemistry, Vol.14(11), W.A. Stubblefield, G.A. Hancock, W.H. Ford, and R.K. Ringer, "Acute and Subchronic Toxicity of Naturally Weathered Exxon Valdez Crude Oil in Mallards and Ferrets." Copyright 1995 SETAC].

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

C1-Phenanthrene/anthracene content in one fresh sample of NSFO (Fuel Oil 5, Chuck Rafkind, National Park Service, Personal Communication, 1996): 2116.3 ng/mg (ppm) (includes both).

C1-Phenanthrene/anthracene content in one sample of groundwater subjected to long term contamination of NSFO (Fuel Oil 5), possibly mixed with some JP-4, motorgas, and JP-8, Colonial National Historical Park Groundwater Site MW-10 (Chuck Rafkind, National Park Service, Personal Communication, 1996): 31,377 ng/L (ppt) (includes both).

Note: the above two PAH concentrations were analyzed by a GC/MS/SIM NOAA protocol [828] modified with methylene chloride extraction for use with water samples (Guy Denoux, Geochemical and Environmental Research Group, Texas A&M University, personal communication 1996).

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 entries for anthracene and phenanthrene.

Laboratory and/or Field Analyses:

The phrase C1-phenanthrene/anthracene refers to a group of alkyl phenanthrene and anthracene compounds which all have one carbon group (that is, one methyl group) attached. Both phenanthrene and anthracene are three-ring PAHs, so all the C1-phenanthrene/anthracenes are three-ring PAHs with one methyl group attached. C1-phenanthrene and C1-anthracene compounds cannot be differentiated with current (1996) analytical techniques.

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 in 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].