ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA

PERYLENE ENTRY

July 1, 1997

COMPILERS/EDITORS:

ROY J. IRWIN, NATIONAL PARK SERVICE

WITH ASSISTANCE FROM COLORADO STATE UNIVERSITY
STUDENT ASSISTANT CONTAMINANTS SPECIALISTS:

MARK VAN MOUWERIK
LYNETTE STEVENS
MARION DUBLER SEESE
WENDY BASHAM

NATIONAL PARK SERVICE
WATER RESOURCES DIVISIONS, WATER OPERATIONS BRANCH
1201 Oakridge Drive, Suite 250
FORT COLLINS, COLORADO 80525

WARNING/DISCLAIMERS:

Where specific products, books, or laboratories are mentioned, no official U.S. government endorsement is intended or implied.

Digital format users: No software was independently developed for this project. Technical questions related to software should be directed to the manufacturer of whatever software is being used to read the files. Adobe Acrobat PDF files are supplied to allow use of this product with a wide variety of software, hardware, and operating systems (DOS, Windows, MAC, and UNIX).

This document was put together by human beings, mostly by compiling or summarizing what other human beings have written. Therefore, it most likely contains some mistakes and/or potential misinterpretations and should be used primarily as a way to search quickly for basic information and information sources. It should not be viewed as an exhaustive, "last-word" source for critical applications (such as those requiring legally defensible information). For critical applications (such as litigation applications), it is best to use this document to find sources, and then to obtain the original documents and/or talk to the authors before depending too heavily on a particular piece of information.

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 uniformed 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).

Perylene (CAS number 198-55-0)

Brief Introduction:

Br.Class: General Introduction and Classification Information:

Perylene is a high molecular weight, 5-ring PAH [697].

Perylene 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].

One of the PAHs found by NASA in 1996 on a rock alleged to be a meteorite from mars (see Uses/Sources section below for details).

Perylene is not universally considered a "pyrogenic" (resulting from high temperatures) PAH or a "petrogenic" (coming from crude oil or oil products) PAH [942].

In sediments perylene can be formed from early diagenesis of plant pigments; it is sometimes considered a geochemical marker for plant pigments such as chlorophyll a, so its presence in sediments is not necessarily indicative of anthropogenic contamination (Gregory Foster, George Mason University, personal communication 1995). Perylene has been said to be one of the few polynuclear aromatic hydrocarbons found in nature [500].

Actually many other PAHs are found in "nature" (see "PAHs as a group" entry), and the statement that perylene is not petrogenic may be premature. Perylene does occur in petroleum products, including:

South LA crude [177],

Fuel Oil 5 (Chuck Rafkind, National Park Service, Personal Communication, 1996),

Sediments contaminated by Diesel Fuel (1D and 2D, (Ray Ahlbrandt, National Park Service, Personal Communication, 1996),

Used Engine Oil [519]:

Br.Haz: General Hazard/Toxicity Summary:

The heavier (4-, 5-, and 6-ring) PAHs, such as this one, are more persistent than the lighter (2- and 3-ring) PAHs and tend to have greater carcinogenic and other chronic impact potential [796].

This is a phototoxic PAH [887,891].

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 compound often occurs 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 compound would be alone (see "PAHs as a group" entry).

Immune Effects:

> All the steps necessary for cellular transformation and cancer induction were demonstrated in cultured human skin fibroblasts: inducible AHH activity, altered cellular proliferation kinetics, and DNA damage [881]. Thus, humans are likely to be susceptible to tumor induction by PAHs by these mechanisms [881]. Carcinogenic PAHs have been suggested to have an effect on immune function, thereby allowing the induction of carcinogenesis, while noncarcinogenic PAHs do not affect immune function [881].
>
> Humoral immunity was monitored in male iron foundry workers in Poland [881]. Coke oven workers (199) were compared to cold-rolling mill workers (76) [881]. The groups were similar with respect to age, length of employment, and smoking habits [881]. The results showed that coke oven workers, exposed to high concentrations of atmospheric PAHs, including fluoranthene, perylene, pyrene, benzo[a]pyrene, chrysene, benz[a]anthracene, dibenz[a,h]anthracene, and benzo[g,h,i]perylene, had reduced levels of serum immunoglobins [881]. The workers most exposed to PAHs worked at the topside area of the coke ovens [881]. Benzo[a]pyrene exposure was used as a reference point [881]. Coke oven workers, exposed to 0.0002-0.50 mg/m3 benzo[a]pyrene, were compared to cold-rolling mill workers, whose exposure to benzo[a]pyrene was 3-5 orders of magnitude less

[881]. Average length of employment was 15 years [881]. IgG, IgA, IgM, and IgE concentrations were measured [881]. Coke oven workers exhibited a marked depression of mean serum IgG and IgA, compared to mill workers [881]. IgM tended to decrease, whereas IgE tended to increase in the coke oven workers [881]. The biological significance of this finding is unclear and is not addressed by the authors [881].

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

No 1995 or 1996 information in EPA IRIS, PRG, RBC sources [868,893,903].

Older reference: Classification of carcinogenicity: 1) evidence in humans: No data; 2) evidence in animals: insufficient. Overall summary evaluation of carcinogenic risk to humans is Group 3: The agent is not classifiable as to its carcinogenicity to humans. /From table/ [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. S7 69 (1987)] [609].

Several other dibenzanthracene-related compounds are considered carcinogens (see dibenzanthracene entry).

This is a phototoxic PAH [887,891]. Although not definitive, phototoxicity represents one clue suggesting possible carcinogenicity.

Amphibians are reported to be quite resistant to PAH carcinogenicity due to their inability to produce mutagenic metabolites of benzo(a)pyrene and perylene [957]. However, PAHs usually occur in the company of other PAHs and the surface eggs and larvae of amphibians, especially those at high altitude, may be prone to acute toxicity impacts from phototoxic properties of mixtures of PAHs (Roy Irwin, National Park Service, personal communication, 1996).

This compound often occurs together with other PAHs, some possibly more carcinogenic (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 this one usually occur in complex mixtures rather than alone. Perhaps the most unambiguous thing that can be said about complex PAH mixtures is that such mixtures are often hazardous in many ways, including carcinogenicity and phototoxicity. (James Huckins, National Biological Survey/USGS, and Roy Irwin, National Park Service, personal communication, 1996).

An investigation of the metabolism of the weak carcinogen, benz(a)anthracene, was compared to that of a group of noncarcinogenic hydrocarbons including benzo(e)pyrene, pyrene, phenanthrene, coronene, triphenylene, and perylene. Male Sprague-Dawley rats were administered sc 0.4 uM doses of these polynuclear aromatic hydrocarbons. Results from HPLC and MS demonstrated that benz(a)anthracene was observed to undergo bioalkylation and biooxidation reactions in rat sc tissue. The other compounds tested did not demonstrate detectable bioalkylation reactions in vivo. These results were consistent with the carcinogenic activity of benz(a)anthracene and the noncarcinogenic potential of the other compounds examined. The data indicated that the metabolic activation of nonfunctional carcinogenic aromatic hydrocarbons was due to the introduction of an alkyl group in a highly reactive mesoanthracenic center in the molecule. Further investigation is necessary to determine whether the bioalkylation reaction can be used as a general probe for the carcinogenic activity of nonfunctional polynuclear aromatic hydrocarbons. (Flesher JW, Myers SR; Drug Metabol Dispos 18, no.2: 163-167, 1990) [609].

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

HSDB Information [609]:

In one study, /perylene/ did not induce mutations in cultured human lymphoblastoid cells. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V32 415 (1983)].

Experimental data: Perylene was tested for carcinogenicity by skin application to mice in one experiment, and no carcinogenic effect was observed. It was also tested in the mouse-skin initiation-promotion assay in one study, with negative results. No data on the teratogenicity of this compound were available. Perylene was mutagenic to Salmonella typhimurium in the presence of exogenous metabolic system. ... The data from one study on chromosomal effects were inadequate to make an evaluation. There is inadequate evidence that perylene is active in short-term tests.

[IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V32 415 (1983)].

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

The heavier (4-, 5-, and 6-ring) PAHs, such as this one, are more persistent than the lighter (2- and 3-ring) PAHs [796].

See "PAHs as a group" entry.

Synonyms/Substance Identification:

Dibenz(de,kl)anthracene [365,609]
peri-Dinaphthalene [365,609]
Perilene [365]

Molecular formula [365]:
$C20-H12$

Associated Chemicals or Topics (Includes Transformation Products):

See also individual entry:

PAHs as a group

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

W.Low (Water Concentrations Considered Low):

No information found.

W.High (Water Concentrations Considered High):

No information found.

W.Typical (Water Concentrations Considered Typical):

Perylene concentrations in water ranged from 0 to 520 ng/L for surface water, 0.1 to 1.4 ng/L for tap water, 0.0 to 1.0 ng/L for rain water, 0 to 0.2 ng/L for subterranean water, and 0.03 to 3.0 ng/L for waste water [847].

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

Cautionary note: This is a phototoxic compound (see more detailed discussion 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]. The reader should be aware that the authors of this document have not yet been able to determine which of the following criteria and benchmarks were developed in the presence or absence of UV light:

For perylene, phototoxicity may be mitigated by degradation [888]. However, alkyl PAHs typically bioconcentrate to a greater degree and degrade more slowly than their parent compounds.

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.

W.Plants (Water Concentrations vs. Plants):

No information found.

W.Invertebrates (Water Concentrations vs. Invertebrates):

No information found.

W.Fish (Water Concentrations vs. Fish):

No information found.

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

No information found.

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

No information found.

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

This is a phototoxic PAH [887,891].

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

Sed.Low (Sediment Concentrations Considered Low):

No information found.

Sed.High (Sediment Concentrations Considered High):

Perylene was detected in 100 % of urban-bay samples from the Puget Sound area. The mean concentration was 53 ug/kg dry weight (ppb), while the median concentration was 27 ug/kg (ppb) [852].

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

Sed.Typical (Sediment Concentrations Considered Typical):

Perylene was detected in 79.2 % of non-urban-bay samples from the Puget Sound area. The mean concentration was 26 ug/kg dry weight (ppb), while the median concentration was 14 ug/kg (ppb) [852].

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

Perylene concentrations in dried sediment from lakes ranged from 4 to 680 ug/kg [847].

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):

NOAA 1990: After studying its own data from the National Status and Trends Program as well as many literature references concerning different approaches to determining sediment criteria, NOAA suggested that there was too little data available to ascertain firm concern levels, but that effects in the two marine studies which were available were associated with the range of 173 ppb dry weight to 1677 ppb dry weight [233]. Anecdotal data showed no effects to invertebrates at 35-85 ppb [233].

Sed.Plants (Sediment Concentrations vs. Plants):

No information found.

Sed.Invertebrates (Sediment Concentrations vs. Invertebrates):

No information found.

Sed.Fish (Sediment Concentrations vs. Fish):

No information found.

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

No information found.

Sed.Human (Sediment Concentrations vs. Human):

No information found.

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.

Soil.High (Soil Concentrations Considered High):

Concentrations of PAH's in bioassay earthworms and bioassay soil from 15 sites at the Times Beach Confined Disposal Facility in Buffalo, N.Y. (1987): The mean concentration of perylene in the soil was 1.2 ppm (dry weight). The range was 0.12-2.8 ppm.

Soil.Typical (Soil Concentrations Considered Typical):

No information found.

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.

Soil.Plants (Soil Concentrations vs. Plants):

No information found.

Soil.Invertebrates (Soil Concentrations vs. Invertebrates):

Concentrations of PAH's in bioassay earthworms and bioassay soil from 15 sites at the Times Beach Confined Disposal Facility in Buffalo, N.Y. (1987): The mean concentration of perylene in the soil was 1.2 ppm (dry weight). The range was 0.12-2.8 ppm. The mean concentration of perylene in the earthworms was 0.30 (ppm ash-free dry weight), the range was 0.036-1.8 ppm [347].

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

No information found.

Soil.Human (Soil Concentrations vs. Human):

No information found.

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.

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

No information found.

Tis.Invertebrates:

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

No information found.

B) Concentrations or Doses of Concern in Food Items

Eaten by Invertebrates:

No information found.

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

Concentrations of PAH's in bioassay earthworms and bioassay soil from 15 sites at the Times Beach Confined Disposal Facility in Buffalo, N.Y. (1987): The mean concentration of perylene in the soil was 1.2 ppm (dry weight). The range was 0.12-2.8 ppm. The mean concentration of perylene in the earthworms was 0.30 (ppm ash-free dry weight), the range was 0.036-1.8 ppm [347].

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.

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

No information found.

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

No information found.

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.

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.

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.

Tis.Human:

A) Typical Concentrations in Human Food Survey Items:

No information found.

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.

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

No information found.

Tis.Misc. (Other Tissue Information):

This is a phototoxic PAH [887,891].

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

Bioconcentration factors (log BCF) are 3.86 for Daphnia pulex, 3.30 for algae, <1.0 for fish, 1.196 for polychaete sp., and -0.398 for capitella capitata [848].

Concentrations of PAH's in bioassay earthworms and bioassay soil from 15 sites at the Times Beach Confined Disposal Facility in Buffalo, N.Y. (1987): The mean concentration of perylene in the soil was 1.2 ppm (dry weight). The range was 0.12-2.8 ppm. The mean concentration of perylene in the earthworms was 0.30 (ppm ash-free dry weight), the range was 0.036-1.8 ppm [347].

Interactions:

No information found.

Uses/Sources:

See also Chem.detail section below for perylene concentrations in various petroleum products.

There are a few polynuclear aromatic hydrocarbons found in nature, such as retene, perylene, and 3,4-benzopyrene [500].

In sediments perylene can be formed from early diagenesis of plant pigments; it is sometimes considered a geochemical marker for plant pigments such as chlorophyll a, so its presence in sediments is not necessarily indicative of anthropogenic contamination

(Gregory Foster, George Mason University, personal communication 1995). Perylene has been said to be one of the few polynuclear aromatic hydrocarbons found in nature [500].

However, the statement that perylene is not petrogenic may be misleading. Perylene does occur in petroleum products, including:

South LA crude [177],

Fuel Oil 5 (Chuck Rafkind, National Park Service, Personal Communication, 1996),

Sediments contaminated by Diesel Fuel (1D and 2D, (Ray Ahlbrandt, National Park Service, Personal Communication, 1996),

Used Engine Oil [519]:

During the summer of 1996, NASA announced that PAHs had been found on a martian meteorite. Three to 6 ring PAHs found included phenanthrene, pyrene, chrysene, perylene, and benzo(a)pyrene, with less than 10% of the mass being alkyl PAHs. It was said that the meteorite PAHs were typified by little alkylation and a lack a dibenzothiophene, making the PAH mixture different than typically found in the earth's atmosphere. However, another unidentified mass of alkyl PAH compounds were also found and NASA acknowledged that PAHs have been found in a wide range of extraterrestrial materials [McKay et.al. 1996, manuscript entitled "Search for Life on Mars: Possible Biogenic Activity in Martian Meteorite ALH84001," a NASA paper available at the time of the NASA press release].

Note from Roy Irwin: This represents and interesting and somewhat speculative attempt to link fingerprinting of PAH combinations to possible life on mars. NASA admits that the PAHs alone do not prove there was life on mars, and I may personally remain a bit skeptical until more comprehensive and convincing evidence is presented.

Major Uses [609]:

Used in the manufacture of organic semiconductors. [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984.,p. V20 676 (1982)].

Forms/Preparations/Formulations:

No information found.

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

Solubilities:

0.00011 mg/L at 20 degrees C to 0.00078 mg/L at 25 degrees C (most values 0.0004) [848].

Virtually insoluble in water (<0.5 ug/l); very sparingly soluble in petroleum ether (a mixture of low-boiling hydrocarbons); slightly soluble in acetone, diethyl ether and ethanol; moderately soluble in benzene; freely soluble in carbon disulphide and chloroform. [IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer,1972-PRESENT. (Multivolume work).,p. V32 412 (1983)] [609].

0.0004 + or - 0.00002 mg/l at 25 deg C in distilled water. [Verschueren, K. Handbook of Environmental Data of Organic Chemicals. 2nd ed. New York, NY: Van Nostrand Reinhold Co., 1983. 968] [609].

Freely soluble in carbon sulfide, chloroform; moderately soluble in benzene; slightly in ether, alcohol, acetone; very sparingly soluble in petroleum ether. Insoluble in water (sic, actually "relatively insoluble". [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989. 1139] [609].

Vapor Pressure [848]:

5.31x10(-9) and 7.00x10(-7) Pa at 25 degrees C.

Henry's Law Constant [848]:

0.440 Pa m(3)/mol

Octanol/Water Partition Coefficient, log Kow [848]:

4.80 to 6.53 (most values near 6.40).

Molecular Weight [609]:

252.30 [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989. 1139].

Density/Specific Gravity [609]:

1.35 [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989. 1139].

Boiling Point:

350-400 (sublimes) [Lide, D.R. (ed). CRC Handbook of Chemistry and Physics. 72nd ed. Boca Raton, FL: CRC Press, 1991-1992.,p. 3-372] [609].

500, 503 degrees C [848].

Melting Point [609]:

273-274 deg C [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989.,p. 1139].

Color/Form [609]:

Yellow to colorless crystals from toluene [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989. 1139].

Golden yellow plates [International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. I&II. Geneva, Switzerland: International Labour Office, 1983. 1758].

Perylene content in one fresh sample of NSFO (Fuel Oil 5, Chuck Rafkind, National Park Service, Personal Communication, 1996): 10.6 ng/mg (ppm).

Perylene 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): 428.6 ng/L (ppt).

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).

Perylene concentrations in Used Engine Oil: 1.1 ppm [519; Reprinted with permission from Environmental Toxicology and Chemistry, Volume 12, Upshall, C., J.F. Payne and J. Hellou, "Induction of MFO enzymes and production of bile metabolites in rainbow trout (Oncorhynchus mykiss) exposed to waste crankcase oil." Copyright 1992 SETAC].

Perylene concentrations in gasolines ranged from 0.01-0.16 mg/kg [847].

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

See Br. Fate section above and "PAHs as a group" entry. No other information found.

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 10 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.

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].

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 (see also: Oil Spill, PAHs, and Petroleum General entries).