3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of PAHs is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of PAHs is located in Table 3-2.

TABLE 3-1. Chemical Identity of Polycyclic Aromatic Hydrocarbons[a]

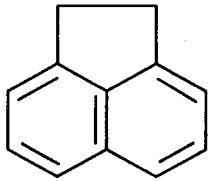
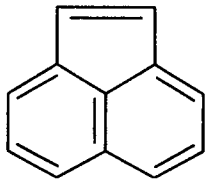
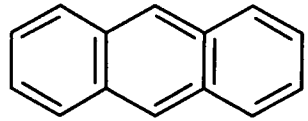
Characteristic	Acenapthene	Acenaphthylene	Anthracene
Synonym(s)	1,2-Dihydroacenaphthylene; 1,8-dihydroacenapthaline; 1,8-ethylenenapthalene; 1,2-dihydroacenapththylene	Cyclopenta[d,e]naphthalene	Anthracin; green oil; paranaphthalene[b]
Registered trade name(s)	No data	No data	Tetra olive NZG; Anthracene oil[d]
Chemical formula	$C_{12}H_{10}$	$C_{12}H_8$	$C_{14}H_{10}$[b]
Chemical structure			
CAS registry	83–29–9	208–96–8	120–12–7[b]
NIOSH RTECS	AB1000000	AB1254000	CA 9350000
EPA hazardous waste	No data	No data	No data
OHM/TADS	8200126	No data	82001222
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	2659	2661	702
NCI	No data	No data	No data

TABLE 3-1. Chemical Identity of Polycyclic Aromatic Hydrocarbons[a] (continued)

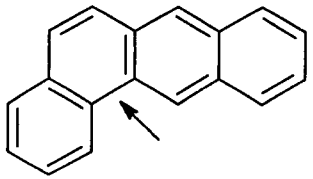
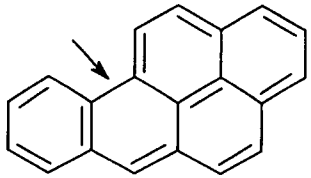
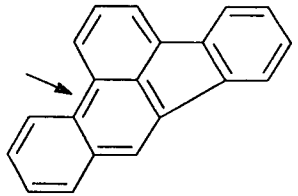
Characteristic	Benzo[a]anthracene	Benzo[a]pyrene	Benzo[b]fluoranthene
Synonym(s)	BA; benz[a]anthracene; 1,2-benzanthracene; benzo[b]-phenanthrene; 2,3-benzophenanthrene; tetraphene[c,d]	Benzo[d,e,f]chrysene; 3,4-benzopyrene, 3,4-benzpyrene; benz[a]pyrene; BP; B[a]P[b]	3,4-Benz[e]acephenanthrylene; 2,3-benzfluoranthene; 3,4-benzfluoranthene; 2,3-benzofluoranthene; 3,4-benzofluoranthene; benzo[e]fluoranthene;B[b]F[b]
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_{18}H_{12}$	$C_{20}H_{12}$[b]	$C_{20}H_{12}$[b]
Chemical structure			
Identification numbers:			
CAS Registry	56–55–3	50–32–8	205–99–2[b]
NIOSH RTECS	CV 9275000[e]	DJ3675000	CU 1400000[e]
EPA Hazardous Waste	U018	U022	No data
OHM/TADS	8200123	No data	8200124[e]
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	4003	2554	4035
NCI	No data	No data	No data

TABLE 3-1. Chemical Identity of Polycyclic Aromatic Hydrocarbons[a] (continued)

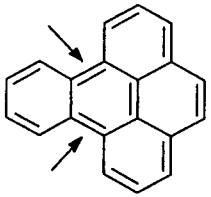
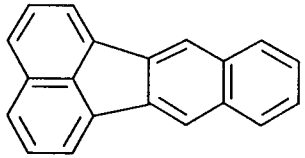
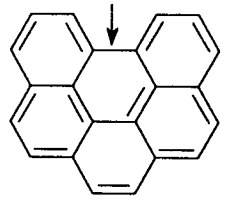
Characteristic	Benzo[e]pyrene	Benzo[k]fluoranthene	Benzo[g,h,i]perylene
Synonym(s)	1.2-Benzopyrene; 1.2-benzpyrene; 4.5 benzopyrene; 4.5-benzpyrene; B[e]P[e]	8.9-Benzfluoranthene; 8.9-benzofluoranthene; 11.12-benzofluoranthene; 2,3,1.8-binaphthylene; dibenzo[b,j,k]fluorene[b]	1,12-Benzoperylene[c]
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_{20}H_{12}$[e]	$C_{20}H_{12}$[b]	$C_{22}H_{12}$[c]
Chemical structure			
CAS registry	192–97–2[e]	207–08–9[b]	191–24–2[c]
NIOSH RTECS	D4500000[e]	DF 350000[e]	DI 6200500[e]
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	8200125[e]	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	4031[e]	6012[e]	6177[e]
NCI	No data	No data	No data

TABLE 3-1. Chemical Identity of Polycyclic Aromatic Hydrocarbons[a] (continued)

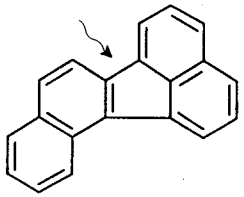
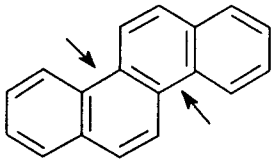
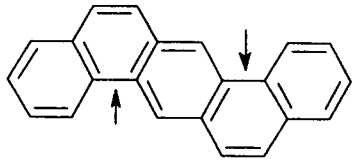
Characteristic	Benzo[j]fluoranthene	Chrysene	Dibenz[a,h]anthracene
Synonym(s)	10.11-Benzofluoranthene; benzo-12.13-fluoranthene; dibenzo[a,j,k]-fluorene; 7.8-benzofluoranthene; B[j]F[e]	1.2-Benzophenanthrene; benzo[a]-phenanthrene; 1,2-benzphenanthrene; benz[a]phenanthrene; 1,2,5,6-dibenzonaphthalene	Dibenz[a,h]anthracene; DB[a,h]A; DBA; 1,2:5,6-dibenz[a]anthracene[b,e]
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_{20}H_{12}$	$C_{18}H_{12}$[b]	$C_{22}H_{14}$[b]
Chemical structure			
CAS registry	205–82–3[e]	218–01–9[b]	53–70–3[b]
NIOSH RTECS	DF 6300000[e]	GC 0700000[e]	HN 2625000[e]
EPA hazardous waste	No data	U050[e]	U063
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	4034[e]	2810	5097
NCI	No data	No data	No data

TABLE 3-1. Chemical Identity of Polycyclic Aromatic Hydrocarbons[a] (continued)

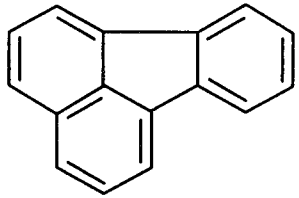
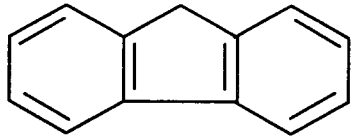
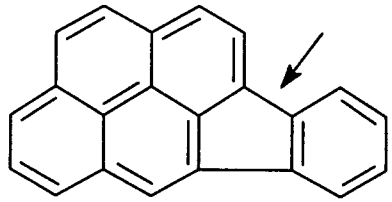
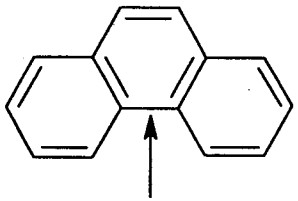
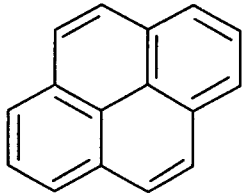
Characteristic	Fluoranthene	Fluorene	Indeno[1,2,3-c,d]pyrene
Synonym(s)	1.2-[1,8-Naphthylene]benzene; 1.2-benzacenaphthene; 1.2-[1.8-naphthalenediyl] benzene; benzo[j,k]fluorene	ortho-Biphenylene methane; diphenylenemethane; 2,2-methylene biphenyl; 2.3-benzidene[b,f]	Indenopyrene; IP; ortho-phenylene pyrene; 1,10-[ortho-phenylene]pyrene; 1,10-[1,2-phenylene]pyrene; 2,3-ortho-phenylene pyrene[b]
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_{16}H_{10}$	$C_{13}H_{10}$[b]	$C_{22}H_{12}$[b]
Chemical structure			
Identification numbers:			
CAS registry	206–44–0	86–73–7[b]	193–39–5[b]
NIOSH RTECS	LL4025000	LL5670000	NK 9300000
EPA hazardous waste	U120	No data	U137
OHM/TADS	8200136	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB	5486	2165	5101
NCI	No data	No data	No data

TABLE 3-1. Chemical Identity of Polycyclic Aromatic Hydrocarbons[a] (continued)

Characteristic	Phenanthrene	Pyrene
Synonym(s)	Phenanthrene; Phenantrin[b]	Benzo[d,e,f]phenanthrene; 8-pyrene[b]
Registered trade name(s)	No data	No data
Chemical formula	$C_{14}H_{10}$[b]	$C_{16}H_{10}$[b]
Chemical structure		
Identification numbers:		
CAS registry	85–01–8[b]	129–00–00[b]
NIOSH RTECS	SF7175000	UR 245000[e]
EPA hazardous waste	No data	No data
OHM/TADS	8200140	No data
DOT/UN/NA/IMCO shipping	No data	No data
HSDB	2166	4023
NCI	No data	No data

[a]All information obtained from HSDB 1994, except where noted.
[b]IARC 1983
[c]Eller 1984
[d]Sax and Lewis 1989
[e]HSDB 1992
[f]Weast et al. 1988

CAS = Chemical Abstracts Service; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; PAHs = polycyclic aromatic hydrocarbons; RTECS = Registry of Toxic Effects of Chemical Substances; ⟶ = bay region; ⇝ = pseudo bay region

TABLE 3-2. Physical and Chemical Properties of Polycyclic Aromatic Hydrocarbons[a]

Property	Acenaphthene	Acenaphthylene	Anthracene
Molecular weight	154.21	152.20	178.2[b]
Color	White	No data	Colorless with violet fluorescence when pure; yellow with green fluorescence when impure
Physical state	Solid (needles)	Solid (prisms/plates)	Solid (tablet or prism)[b]
Melting point	95 °C	92–93 °C	218 °C[b]
Boiling point	96.2 °C	265–275 oC	342 °C[b], 340 °C[e]
Density at 20/4 °C	1.225 g/cm^3 at 0 °C	No data	No data
Specific gravity	1.0242 at 90 °C/4 °C[e]	0.8988 at 16 °C/2 °C	1.25 at 27 °C/4 °C; 1.283 at 25 °C/4 °C[e]
Odor	No data	No data	Weak aromatic odor
Odor threshold:			
Water	0.08 ppm	No data	No data
Air	0.08 ppm	No data	No data
Solubility:			
Water	1.93 mg/L[p]	3.93 mg/L water	0.076 mg/L[p]
Organic solvents	Soluble in alcohol, methanol, propanol, chloroform, benzene, toluene, glacial acetic acid	Alcohol, ether, benzene	Acetone; benzene, carbon disulphide, carbon tetrachloride, chloroform, ether, ethanol, methanol, toluene[e,b]
Partition coefficients:			
Log K_{ow}	3.98[k]	4.07[k]	4.45[k]
Log K_{oc}	3.66[k]	1.40[k]	4.15[k]
Vapor pressure	4.47x10^{-3} mm Hg[m]	0.029 mm Hg at 20 °C[k]	1 mm Hg at 145 °C[b]; 1.7x10^{-5} mm Hg at 25 °C[k]
Henry's law constant	7.91x10^{-5} atm-^{3}/mol[r]	1.45x10^{-3} atm-m^3/mol	1.77x10^{-5} atm-m^3/mol[r]
Autoignition temperature	No data	No data	540 °C[i]
Flashpoint	No data	No data	121 °C(closed cup)[d]
Flammability limits	Dust is moderately flammable[n]	No data	No data
Conversion factors	0	0	0
Explosive limits	No data	No data	Lower, 0.6% by volume[d]

TABLE 3-2. Physical and Chemical Properties of Polycyclic Aromatic Hydrocarbons[a] (continued)

Property	Benzo[a]anthracene	Benzo[a]pyrene	Benzo[b]fluoranthene
Molecular weight	228.29[c]	252.3[b]	252.3[b]
Color	Yellow-blue fluorescence[e]	Pale yellow	Colorless
Physical state	Solid (plates)	Solid (plates or needles)[f]	Solid (needles)[e] (recrystallized from benzene/ligroin)
Melting point	158–159 °C[c]; 162 °C[e]	179–179.3 °C[f]	168.3 °C[b]
Boiling point	400 °C[i]; 435 °C sublimes[f]	310–312 °C at 10 mm Hg[f]; 495 °C[j]	No data
Density	1.274 g/cm^3 at 20 °C	1.351 g/cm^{3,h}	No data
Specific gravity	No data	No data	No data
Odor	No data	Faint aromatic odor	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	0.010 mg/L[p]	2.3x10^{-3} mg/L[p]	0.0012 mg/L[q]
Organic solvents	Slightly soluble in acetic acid and hot ethanol; soluble in acetone and diethyl ether; very soluble in benzene[b]	Sparingly soluble in ethanol and methanol; soluble in benzene, toluene, xylene, and ether	Slightly soluble in benzene, acetone[b]
Partition coefficients:			
Log K_{ow}	5.61[k]	6.06[k]	6.04[k]
Log K_{oc}	5.30[k]	6.74[k]	5.74[k]
Vapor pressure	2.2x10^{-8} mm Hg at 20 °C	5.6x10^{-9} mm Hg[k]	5.0x10^{-7} mm Hg at 20–25 °C[r]
Henry's law constant	1x10^{-6} atm–m^3/mol	4.9x10^{-7} atm-m^3/mol[k]	1.22x10^{-5} atm-m^3/mol[k]
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors	0	0	0
Explosive limits	No data	No data	No data

TABLE 3-2. Physical and Chemical Properties of Polycyclic Aromatic Hydrocarbons[a] (continued)

Property	Benzo[e]pyrene	Benzo[k]fluoranthene	Benzo[g,h,i]perylene
Molecular weight	252.30[d]	252.3	276.34[c]
Color	Colorless[b]	Pale yellow	Pale yellow-green
Physical state	Prisms or plates (recrystallized from benzene)[g]	Solid (needles)	Solid (plate)
Melting point	178–179 °C[d]	215.7 °C	273 °C[c]
Boiling point	310–312 °C at 10 mm Hg[g]	480 °C	550 °C
Density	No data	No data	No data
Specific gravity	No data	No data	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	6.3×10^{-3} mg/L at 25 °C[d]	7.6×10^{-4} mg/L at 25 °C	2.6×10^{-4} mg/L at 25 °C
Organic solvents	Acetone[g]	Soluble in benzene, acetic acid, ethanol[b]	Soluable in benzene, dichloromethane, acetone[g]
Partition coefficients:			
Log K_{ow}	No data	6.06[k]	6.50[k]
Log K_{oc}	No data	5.74[k]	6.20[k]
Vapor pressure	5.7×10^{-9} mm Hg at 25 °C[d]	9.59×10^{-11} mm Hg	1.03×10^{-10} mm Hg at 25 °C[k]
Henry's law constant	No data	3.87×10^{-5} atm–m^3/mol[k]	1.44×10^{-7} atm-m^3/mol[k]
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors	0	0	0
Explosive limits	No data	No data	No data

TABLE 3-2. Physical and Chemical Properties of Polycyclic Aromatic Hydrocarbons[a] (continued)

Property	Benzo[j]fluoranthene	Chrysene	Dibenz[a,h]anthracene
Molecular weight	252.32[d]	228.3[b]	278.35[c]
Color	Yellow or orange[d]	Colorless with blue or red-blue fluorescence[b,e]	Colorless[b]
Physical state	Plates (recrystallized from ethanol) or needles (recrystallized from acetic acid)[d,h]	Solid (plates)[e]	Solid (plates or leaftlets)[e]
Melting point	166 °C[d]	255–256 °C[b]	262 °C[c]
Boiling point	No data	448 °C[b]	No data
Density	No data	No data	1.282 g/cm^3[,h]
Specific gravity	No data	1.274 at 20 °C/4 °C[i]	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	6.76x10^{-3} mg/L at 25 °C[d]	2.8x10^{-3} mg/L[p]	5x10^{-4} mg/L[b]
Organic solvent(s)	Slightly soluble in alcohol and acetic acid; soluble in hydrogen sulfide on heating[d]	Slightly soluble in acetone, carbon disulphide, diethyl ether, ethanol glacial acetic acid toluene hot xylene; soluble in benzene[b]	Slightly soluble in ethyl alcohol; soluble in acetone, acetic acid, benzene, toluene and xylene[e]
Partition coefficients:			
Log K_{ow}	6.12[d]	5.16[k]	6.84[k]
Log K_{oc}	4.7–4.8[d]	5.30[k]	6.52[k]
Vapor pressure	1.50x10^{-8} mm Hg at 25 °C[d]	6.3x10^{-7} mm Hg at 25 °C[k]	1x10^{-10} mm Hg at 20 °C[k]
Henry's law constant	1x10^{-6} atm–m^3/mol[d]	1.05x10^{-6} atm-m^3/mol[k]	7.3x10^{-8} atm-m^3/mol[k]
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors	0	0	0
Explosive limits	No data	No data	No data

TABLE 3-2. Physical and Chemical Properties of Polycyclic Aromatic Hydrocarbons[a] (continued)

Property	Fluoranthene	Fluorene	Indeno[1,2,3-c,d]pyrene
Molecular weight	202.26	166.2[g]	276.3[g]
Color	Pale yellow	White[g]	Yellow plates or needles showing a greenish-yellow fluorescence[g]
Physical state	Solid (needles or plates)	Solid (leaflets or flakes; crystalline plates)[g]	Solid (plates or needles)[g]
Melting point	11 °C	116–117 °C[g]	163.6 °C[g]
Boiling point	~375 °C	295 °C[g]	530 °C
Density	No data	No data	No data
Specific gravity	1.252 at 0 °C/4 °C	1.203 at 0 °C/4 °C	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	0.20–0.26 mg/L[g]	1.68–1.98 mg/L[g]	0.062 mg/L[g]
Organic solvents	Alcohol, ether, benzene, acetic acid	Acetic acid, acetone, benzene, carbon disulphide, carbon tetrachloride, diethyl ether, ethanol, pyrimidine, solution, toluene[g]	Soluble in organic solvents[g]
Partition coefficients:			
Log K_{ow}	4.90[k]	4.18[k]	6.58[k]
Log K_{oc}	4.58[k]	3.86[k]	6.20[k]
Vapor pressure	5.0×10^{-6} mm Hg at 25 °C[k]	3.2×10^{-4} mm Hg at 20 °C[d]	$\sim 10^{-11}$–10^{-6} mm Hg at 20 °C[k]
Henry's law constant	6.5×10^{-6} atm–m^3/mol[k]	1.0×10^{-4} atm-m^3/mol[r]	6.95×10^{-8} atm-m^3/mol[k]
Autoignition temperature	No data	No data	No data
Flashpoint	No data	No data	No data
Flammability limits	No data	No data	No data
Conversion factors	0	0	0
Explosive limits	No data	No data	No data

TABLE 3-2. Physical and Chemical Properties of Polycyclic Aromatic Hydrocarbons[a] (continued)

Property	Phenanthrene	Pyrene
Molecular weight	178.2[b]	202.3[b]
Color	Colorless[b]	Colorless, pale yellow plates (recrystallized from toluene) or slight blue fluorescence (recrystallized from ethanol or sublimation)[b]
Physical state	Solid (plates, crystals, or leaflets)[b]	Solid (plates or tablets)[b]
Melting point	100 °C[b]	156 °C
Boiling point	340 °C	393 °C[e]; 404 °C[l]
Density	0.980 g/cm^3 at 4 °C	1.271 g/cm^3 at 23 °C
Specific gravity	No data	1.271 at 23 °C/4 °C
Odor	Faint aromatic odor	No data
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water at 25 °C	1.20 mg/L[p]	0.077 mg/L[p]
Organic solvents	Soluble glacial acetic acid, benzene, carbon disulphide, carbon tetrachloride, anhydrous diethyl ether, ethanol, toluene[b]	Soluble in alcohol benzene, carbon disulphide, diethyl ether, ethanol, petroleum ether, toluene, race tone[b]
Partition coefficients:		
Log K_{ow}	4.45[k]	4.88[k]
Log K_{oc}	4.15[k]	4.58[k]
Vapor pressure	6.8x10^{-4} mm Hg at 25 °C[d]	2.5x10^{-6} mm Hg at 25 °C[k]
Henry's law constant	2.56x10^{-5} atm–m^3/mol[r]	1.14x10^{-5} atm-m^3/mol[r]
Autoignition temperature	No data	No data
Flashpoint	No data	No data
Flammability limits	No data	No data
Conversion factors	0	0
Explosive limits	No data	No data

[a]All information obtained from HSDB except where noted
[b]IARC 1973
[c]Eller 1984
[d]HSDB 1994
[e]Weast et al. 1988
[f]Weast 1987
[g]IARC 1983
[h]Temperature not specified
[i]Sax and Lewis 1989
[j]Aldrich 1986
[k]Mabey et al. 1982
[l]Windholz 1983
[m]EPA 1987a
[n]ITII 1982
[p]Yalkowsky et al 1993
[q]Sims and Overcash 1983
[r]Nirmalakhandan and Speece 1988

The following equation can be used for the converstion of vapor phase PAHs at 25 °C:

$$\frac{\text{mg/m}^3 \times 24.45}{\text{Mol. wt.}}$$