REFERENCE 5

2.2 Physical and chemical properties

Physical and chemical properties relevant to the toxicological and ecotoxicological evaluation of the PAH are summarized in Table 4. It should be kept in mind that the values for any one parameter may be derived from different sources, with different methods of measurement or calculation, so that individual values cannot be compared directly unless the original sources are consulted. In particular, the vapour pressures reported in the literature for the same PAH vary by up to several orders of magnitude (Mackay & Shiu, 1981; Lane, 1989). Variations are also seen in the reported solubility in water of various PAH, although the values are generally within one order of magnitude (National Research Council Canada, 1983). Flash-points were available only for three compounds with high molecular mass (for naphthalene, 78.9°C by the open-cup method and 87.8°C by the closed-cup method; anthracene, 121°C by the closed-cup method; and phenanthrene, 171°C by the open-cup method). Explosion limits were available only for naphthalene (0.9–5.9 vol %) and ananthrone (0.6 vol %) (Lewis, 1992). Vapour density (air = 1) was 4.42 for naphthalene (IARC, 1973), 5.32 for acenaphthene, 6.15 for anthracene (Lewis, 1992), 6.15 for phenanthrene, and 8.7 for benzo[*a*]pyrene (National Institute for Occupational Safety and Health and Occupational Safety and Health Administration, 1981).

The physical and chemical properties are largely determined by the conjugated alpha-electron systems, which vary fairly regularly with the number of rings and molecular mass, giving rise to a more or less wide range of values for each parameter within the whole class. At room temperature, all PAH are solids. The general characteristics common to the class are high melting- and boiling-points, low vapour pressure, and very low solubility in water. PAH are soluble in many organic solvents (IARC, 1983; Agency for Toxic Substances and Disease Registry, 1990; Lide, 1991) and are highly lipophilic.

Vapour pressure tends to decrease with increasing molecular mass, varying by more than 10 orders of magnitude. This characteristic affects the adsorption of individual PAH onto particulate matter in the atmosphere and their retention on particulate matter during sampling on filters (Thrane & Mikalsen, 1981). Vapour pressure increases markedly with ambient temperature (Murray et al., 1974), which additionally affects the distribution coefficients between gaseous and particulate phases (Lane, 1989). Solubility in water tends to decreases with increasing molecular mass. For additional information, refer to section 4.1.

PAH are chemically inert compounds (see also section 4.4). When they react, they undergo two types of reaction: electrophilic substitution and addition. As the latter destroys the aromatic character of the benzene ring that is affected, PAH tend to form derivatives by the former reaction; addition is often followed by elimination, resulting in net substitution. The chemical and photochemical reactions of PAH in the atmosphere have been reviewed

Table 4. Physical and chemical properties of polycyclic aromatic compounds covered in this monograph, ranked by molecular mass

Compound	Colour	Melting-point[a] (°C)	Boiling-point (°C)	Vapour pressure (Pa at 25°C)	Density[c]	n-Octanol: water partition coefficient (log K_{ow})	Solubility in water at 25°C (µg/litre)[d]	Henry's law constant at 25°C (kPa)
Naphthalene	White[b]	81	217.9[a]	10.4[g]	1.154[25 h]	3.4[j]	3.17 x 10^4	4.99 x 10^{-2} [k]
Acenaphthylene		92–93		8.9 x 10^{-1} [g]	0.899[16/2 h]	4.07[f]		114 x 10^{-3} [l]
Acenaphthene	White[b]	95	279[h]	2.9 x 10^{-1} [g]	1.024[90/4 h]	3.92[f]	3.93 x 10^3	1.48 x 10^{-2} [k]
Fluorene	White[e]	115–116	295[e]	9.8 x 10^{-2} [g]	1.203[0/4 h]	4.18[m]	1.98 x 10^3	1.01 x 10^{-2} [n]
Anthracene	Colourless[c]	216.4	342[e]	8.0 x 10^{-4} [g]	1.283[25/4 h]	4.5[j]	73	7.3 x 10^{-2} [n]
Phenanthrene	Colourless[p]	100.5	340[h]	1.6 x 10^{-2} [g]	0.980[4 h]	4.6[j]	1.29 x 10^3	3.98 x 10^{-3} [k]
1-Methylphenanthrene		123	354–355[v]			5.07[s]	255 (24°C)[t]	
Fluoranthene	Pale yellow[h]	108.8	375[h]	1.2 x 10^{-3} [g]	1.252[0/4 h]	5.22[u]	260	6.5 x 10^{-4} (20 °C)[w]
Pyrene	Colourless[e]	150.4	393[h]	6.0 x 10^{-4} [g]	1.271[23/4 h]	5.18[j]	135	1.1 x 10^{-3} [n]
Benzo[a]fluorene	Colourless[x]	189–190[h]	399–400[y]			5.32[z]	45	
Benzo[b]fluorene	Colourless[x]	213.5	401–402[y]		1.226[aa]	5.75[x]	2.0	
Benzo[ghi]fluoranthene	Yellow[bb]	128.4	432[cc]		1.345[23 dd]			
Cyclopenta[cd]pyrene	Orange[x]	170	439[cc]					
Benz[a]anthracene	Colourless[b]	160.7	400[b]	2.8 x 10^{-5} [g]	1.226[aa]	5.61[f]	14	
Benzo[c]phenanthrene	Colourless[x]	66.1			1.265[ff]			
Chrysene	Colourless with blue fluorescence[b]	253.8	448[h]	8.4 x 10^{-5} (20°C)[gg]	1.274[20/4 a]	5.91[u]	2.0	
Triphenylene	Colourless[x]	199	425[bb]		1.3[p]	5.45[hh]	43	
5-Methylchrysene	Colourless[x]	117.1	459[ii]				62 (27°C)[jj]	
Benzo[b]fluoranthene	Colourless[i]	168.3	481[kk]	6.7 x 10^{-5} (20°C)[gg]		6.12[f]	1.2[ll] (20°C)[u]	5.1 x 10^{-5}
Benzo[j]fluoranthene	Yellow[b]	165.4	480[cc]	2.0 x 10^{-6} [i]		6.12[mm]	2.5[nn]	

Table 4. (continued)

Compound	Colour	Melting-point[a] (°C)	Boiling-point (°C)	Vapour pressure (Pa at 25°C)	Density[c]	n-Octanol: water partition	Solubility in water at 25°C (µg/litre)[d]	Henry's law constant at 25°C (kPa)

						coefficient (log Kow)		
Benzo[k]fluoranthene	Pale yellow[h]	215.7	480[h]	1.3×10^{-8} (20°C)[oo]		6.84[ss]	0.76[f]	4.4×10^{-5} (20°C)[w]
Benzo[a]pyrene	Yellowish[e]	178.1	496[kk]	7.3×10^{-7}[oo]	1.351[pp]	6.50[u]	3.8	3.4×10^{-5} (20°C)
Benzo[e]pyrene	Pale yellow[x]	178.7	493[kk]	7.4×10^{-7}[qq]		6.44[rr]	5.07 (23°C)[tt]	
Perylene	Yellow to colourless[q]	277.5	503[aa]		1.35[v]	5.3[uu]	0.4	
Anthanthrene	Golden yellow[bb]	264	547[yy]		1.39[v]			
Benzo[ghi]perylene	Pale yellow-green[bb]	278.3	545[ii]	1.4×10^{-8} [ww]	1.329[20] [kk]	7.10[u]	0.26	2.7×10^{-5} (20°C)[u]
Indeno[1,2,3-cd]pyrene	Yellow[i]	163.6	536[yy]	1.3×10^{-8} (20°C)[qq]		6.50[f]	62[f]	2.9×10^{-5} (20°C)[v]
Dibenz[a,h]anthracene	Colourless[i]	266.6	524[yy]	1.3×10^{-8} (20°C)	1.282[i]	6.50[zz]	0.5 (27°C)[jj]	7 x 10^{-6} [ll]
Coronene	Yellow[h]	439	525[aaa]	2.0×10^{-10} [qq]	1.37[h]		5.4[uu]	0.14
Dibenzo[a,e]pyrene	Pale yellow[h]	244.4	592[vv]					
Dibenzo[a,h]pyrene	Golden yellow[i]	317	596[vv]					
Dibenzo[a,i]pyrene	Greenish-yellowish[i]	202	594[vv]	3.2×10^{-10} [mm]		7.30[hh]	0.17[i]	4.31×10^{-6} [ll]
Dibenzo[a,l]pyrene	Pale yellow[i]	162.4	595[vv]					

[a] From Karcher et al. (1985); Karcher (1988)
[b] From Lewis (1992)
[c] When two temperatures are given as superscripts, they indicate the specific gravity, i.e. the density of the substance at the first reported temperature relative to the density of water at the second reported temperature. When there is no value, or only one, for temperature, the datum is in grains per millilitre, at the indicated temperature, if any.

Table 4 (continued)

[d] From Mackay & Shiu (1977), except where noted
[e] From Budavari (1989)
[f] From National Toxicology Program (1993)
[g] From Sonnefeld et al. (1983)
[h] From Lide (1991)
[i] From IARC (1977)
[j] From Karickhoff et al. (1979)
[k] From Mackay et al. (1979)
[l] Calculated by Syracuse Research Center; from National Toxicology Program (1993)
[m] Calculated as per Lee et al. (1971); from US Environmental Protection Agency (1980)
[n] From Mackay & Shiu (1981)
[o] When pure, colourless with violet fluorescence; from Budavari (1989)
[p] From Rawley (1987)
[q] From National Institute for Occupational Safety and Health and Occupational Safety and Health Administration (1981)
[r] From Kruber & Marx (1938)
[s] Calculated by Karcher et al. (1991)
[t] From May et al. (1978)
[u] From Bruggeman et al. (1982)
[v] At ambient temperature; from Inokuchi & Nakagaki (1959)
[w] From Ten Hulscher et al. (1992)
[x] Personal observation by J. Jacob, Germany, on high-purity, certified reference materials
[y] From Kruber (1937)
[z] Calculated by Miller et al. (1985)
[aa] From Schuyer et al. (1953)
[bb] From IARC (903)
[cc] From Kruber & Grigoleit (1954)
[dd] From Ehrlich & Beevers (1956)
[ee] Reported by Grimmer (1983a)
[ff] From Beilstein Institute for Organic Chemistry (1993)
[gg] Reported by Sims & Overcash (1983)
[hh] Calculated by Yalkowsky & Valvani (1979)
[ii] Calculated by White (1986)
[jj] From Davis et al. (1942)
[kk] From review by Bjorseth (1983); original references cited by White (1986)
[ll] Temperature not given; reported by Sims & Overcash (1983)
[mm] Calculated by National Toxicology Program (1993)
[nn] Temperature not given; unpublished result cited by Wise et al. (1981)
[oo] From US Environmental Protection Agency (1980)

Table 4 (continued)

[pp] From Kronberger & Weiss (1944)
[qq] From review of Santodonato et al. (1981)
[rr] Calculated by Ruepert et al. (1985)
[ss] From Verschueren (1983)
[tt] From Schwarz (1977)
[uu] From Brooke et al. (1986)
[vv] From Agency for Toxic Substances and Disease Registry (1990)
[ww] From White (1948)
[yy] Estimated from gas chromatographic retention time; from Grimmer (1983a)
[zz] From Means et al. (1980)
[aaa] From Von Boente (1985)