

## APPENDIX

### CHEMICAL AND PHYSICAL DATA FOR SOME NON-HETEROCYCLIC POLYCYCLIC AROMATIC HYDROCARBONS

The molecular formulae and relative molecular masses of these compounds are given in Table 1. Their structural formulae are given in Figure 1 and their selected physical and chemical properties are summarized in Table 2.

#### 1. Acenaphthene

##### 1.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 83-32-9

*Chem. Abstr. Name:* Acenaphthene

*IUPAC Systematic Name:* Acenaphthene

*Synonyms:* 1,8-dihydroacenaphthene; 1,2-dihydroacenaphthylene; 1,8-ethylene-naphthalene; peri-ethylenenaphthalene; naphthyleneethylene

##### 1.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006) unless otherwise specified

(a) *Description:* Orthorhombic bipyramidal needles from alcohol

(b) *Boiling-point:* 279 °C

(c) *Melting-point:* 95 °C

(d) *Density:* 1.189

(e) *Spectroscopy data:* ultraviolet (UV)/visible (VIS), infrared, fluorescence, mass and nuclear magnetic resonance (NMR) spectral data have been reported (Karcher *et al.*, 1988; NIST, 2005).

(f) *Water solubility:* 3.9 mg/L at 25 °C (Miller *et al.*, 1985)

(g) *Vapour pressure:* 0.29 Pa at 25 °C (Sonnefeld *et al.*, 1983)

(h) *Log K<sub>ow</sub> (octanol-water):* 3.92 (Sangster Research Laboratories, 2005)

- (i) *Henry's law constant*: 18.5 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)
- (j) *Atmospheric OH rate constant*:  $8.0 \pm 0.4 \times 10^{-11}$  cm<sup>3</sup>/mol/s (Reisen & Arey, 2002)

## 2. Acepyrene

### 2.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 25732-74-5

*Chem. Abstr. Name*: Cyclopenta[cd]pyrene, 3,4-dihydro-

*IUPAC Systematic Name*: 3,4-Dihydrocyclopenta[cd]pyrene

*Synonyms*: 2,3-Acepyrene\* ; 3,4-dimethylenepyrene

\*Alternative numbering convention

### 2.2 Chemical and physical properties of the pure substance

- (a) *Description*: White crystals (Tintel *et al.*, 1983)
- (b) *Melting-point*: 133–134 °C (Tintel *et al.*, 1983; Otero-Lobato, 2005)
- (c) *Spectroscopy data*: NMR (Tintel *et al.*, 1983; Otero-Lobato *et al.*, 2005), UV, infrared and mass spectral data have been reported (Tintel *et al.*, 1983; NIST, 1998)

## 3. Anthanthrene

### 3.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 191-26-4

*Chem. Abstr. Name*: Dibenzo[def,mno]chrysene

*IUPAC Systematic Name*: Dibenzo[def,mno]chrysene

*Synonym*: Dibenzo[cd,jk]pyrene

### 3.2 Chemical and physical properties of the pure substance

- (a) *Description*: Golden yellow plates (recrystallized from xylene) (Clar, 1964)
- (b) *Melting-point*: 264 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Log K<sub>ow</sub> (octanol–water)*: 7.04 (Howard & Meylan, 1997; Sangster Research Laboratories, 2005)

## 4. Anthracene

### 4.1 Nomenclature

*Chem. Abstr. Services Reg. No.:* 120-12-7

*Chem. Abstr. Name:* Anthracene

*IUPAC Systematic Name:* Anthracene\*

*Synonyms:* Anthracin; paranaphthalene

\*Numbering exception

### 4.2 Chemical and physical properties of the pure substance

From O'Neil (2006), unless otherwise specified

- (a) *Description:* Monoclinic plates from alcohol. When pure, colourless with violet fluorescence; when impure (due to tetracene, naphthacene), yellow with green fluorescence
- (b) *Boiling-point:* 342 °C
- (c) *Melting-point:* 218 °C; 216.4 °C (Karcher *et al.*, 1985; Lide, 2005)
- (d) *Density:* 1.25 at 27 °C relative to water at 4 °C; 1.283 at 25 °C relative to water at 4 °C (Lide, 2005)
- (e) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (f) *Water solubility:* 0.0436 at 25 °C (May *et al.*, 1983)
- (g) *Vapour pressure:*  $8.0 \times 10^{-4}$  Pa at 25 °C (Sonnefeld *et al.*, 1983)
- (h) *Log  $K_{ow}$  (octanol-water):* 4.45 (Howard & Meylan, 1997); 4.54 (Miller *et al.*, 1985)
- (i) *Henry's law constant:* 5.64 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)

## 5. 11H-Benz[bc]aceanthrylene

### 5.1 Nomenclature

*Chem. Abstr. Services Reg. No.:* 202-94-8

*Chem. Abstr. Name:* 11H-Benz[bc]aceanthrylene

*IUPAC Systematic Name:* 11H-Benz[bc]aceanthrylene

*Synonyms:* Benz[a]anthracene, 1,12-methylene-; 1',9-methylene-1,2-benzanthracene

### 5.2 Chemical and physical properties of the pure substance

- (a) *Melting-point:* 123 °C (Ray & Harvey, 1983); 120.5-121 °C (Harvey *et al.*, 1991)
- (b) *Spectroscopy data:* NMR (Ray & Harvey, 1983) and UV/VIS (Harvey *et al.*, 1991) spectra have been reported.

## 6. Benz[j]aceanthrylene

### 6.1 Nomenclature

*Chem. Abstr. Services Reg. No.:* 202-33-5

*Chem. Abstr. Name:* Benz[j]aceanthrylene

*IUPAC Systematic Name:* Benz[j]aceanthrylene

*Synonyms:* Benz[7,8]aceanthrylene; cholanthrylene; naphth[2,1-*d*]acenaphthylene

### 6.2 Chemical and physical properties of the pure substance

From Sangaiah *et al.* (1983)

(a) *Description:* Orange plates from hexane

(b) *Melting-point:* 170–171 °C

(c) *Spectroscopy data:* UV/VIS, mass and NMR spectral data have been reported.

## 7. Benz[l]aceanthrylene

### 7.1 Nomenclature

*Chem. Abstr. Services Reg. No.:* 211-91-6

*Chem. Abstr. Name:* Benz[l]aceanthrylene

*IUPAC Systematic Name:* Benz[l]aceanthrylene

*Synonym:* Naphth[1,2-*d*]acenaphthylene

### 7.2 Chemical and physical properties of the pure substance

From Sangaiah *et al.* (1983)

(a) *Melting-point:* 157–158 °C

(b) *Spectroscopy data:* UV/VIS, mass and NMR spectral data have been reported.

## 8. Benz[a]anthracene

### 8.1 Nomenclature

*Chem. Abstr. Services Reg. No.:* 56-55-3

*Chem. Abstr. Name:* Benz[a]anthracene

*IUPAC Systematic Name:* Benz[a]anthracene

*Synonyms:* 1,2-Benz[a]anthracene; benzanthracene; 1,2-benzanthracene; benzanthrene; 1,2-benzanthrene; benzo[a]anthracene; benzoanthracene; 1,2-benzoanthracene; benzo[b]phenanthrene; 2,3-benzophenanthrene; tetraphene

## 8.2 Chemical and physical properties of the pure substance

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Plates from glacial acetic acid or alcohol with greenish-yellow fluorescence
- (b) *Melting-point*: 160.7 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility*: 0.0090 mg/L at 25 °C (May *et al.*, 1983)
- (e) *Vapour pressure*:  $2.8 \times 10^{-5}$  Pa at 25 °C (Sonnenfeld *et al.*, 1983)
- (f) *Log  $K_{ow}$  (octanol–water)*: 5.91 (Miller *et al.*, 1985; Sangster Research Laboratories, 2005)
- (g) *Henry's law constant*: 1.22 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)

## 9. Benzo[b]chrysene

### 9.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 214-17-5

*Chem. Abstr. Name*: Benzo[b]chrysene

*IUPAC Systematic Name*: Benzo[b]chrysene

*Synonyms*: 2,3-Benzochrysene; benzo[c]tetraphene; 3,4-benzotetraphene; 1,2:6,7-dibenzophenanthrene; 2,3:7,8-dibenzophenanthrene<sup>\*</sup>; naphth[2,1-a]anthracene

<sup>\*</sup>Alternative numbering convention

### 9.2 Chemical and physical properties of the pure substance

- (a) *Description*: Pale green-yellow leaves from xylene (Lide, 1992)
- (b) *Melting-point*: 294 °C (Lide, 1992); 299.7 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Log  $K_{ow}$  (octanol–water)*: 7.11 (Sangster Research Laboratories, 2005)

## 10. Benzo[g]chrysene

### 10.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 196-78-1

*Chem. Abstr. Name*: Benzo[g]chrysene

*IUPAC Systematic Name*: Benzo[g]chrysene

*Synonyms*: Benzo[a]triphenylene; 1,2:3,4-dibenzophenanthrene; 1,2,3,4-dibenzophenanthrene; 1,2:3,4:7,8-tribenznaphthalene

## 10.2 *Chemical and physical properties of the pure substance*

- (a) *Melting-point*: 116 °C (Sukumaran & Harvey, 1981); 114 °C (Agarwal *et al.*, 1985); 112–114 °C (Utermoehlen *et al.*, 1987)
- (b) *Spectroscopy data*: Mass and NMR spectral data have been reported (Sukumaran & Harvey, 1981; Agarwal *et al.*, 1985).

## 11. **Benzo[*a*]fluoranthene**

### 11.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 203-33-8

*Chem. Abstr. Name*: Benz[*a*]aceanthrylene

*IUPAC Systematic Name*: Benz[*a*]aceanthrylene

*Synonyms*: 1,2-Benzfluoranthene; benzo[*a*]aceanthrylene; 1,2-benzofluoranthene; dibenzo[*c,lm*]fluorene

### 11.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Golden needles from petroleum ether (Cho & Harvey, 1987a)
- (b) *Melting-point*: 146.3 °C (Karcher *et al.*, 1985); 143-145 °C (Cho & Harvey, 1987a)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; Cho & Harvey, 1987b)

## 12. **Benzo[*b*]fluoranthene**

### 12.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 205-99-2

*Chem. Abstr. Name*: Benz[*e*]acephenanthrylene

*IUPAC Systematic Name*: Benz[*e*]acephenanthrylene

*Synonyms*: 3,4-Benz[*e*]acephenanthrylene\* ; 2,3-benzfluoranthene; 3,4-benzfluoranthene\* ; benzo[*e*]fluoranthene; 3,4-benzofluoranthene\*

\*Alternative numbering convention

### 12.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Needles from benzene (Lide, 2005)
- (b) *Melting-point*: 168 °C (Lide, 2005); 168.3 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility*: 0.0015 mg/L (Howard & Meylan, 1997)
- (e) *Log K<sub>ow</sub> (octanol–water)*: 5.78 (Sangster Research Laboratories, 2005)

(f) *Henry's law constant*: 0.051 Pa m<sup>3</sup>/mol at 20 °C (ten Hulscher *et al.*, 1992)

### 13. Benzo[ghi]fluoranthene

#### 13.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 203-12-3

*Chem. Abstr. Name*: Benzo[ghi]fluoranthene

*IUPAC Systematic Name*: Benzo[ghi]fluoranthene

*Synonyms*: 2,13-Benzofluoranthene<sup>\*</sup>; 7,10-benzofluoranthene<sup>\*</sup>; benzo[*mno*]fluoranthene

<sup>\*</sup>Alternative numbering convention

#### 13.2 Chemical and physical properties of the pure substance

(a) *Description*: Yellow needles with greenish-yellow fluorescence (recrystallized from petroleum ether); blue fluorescence in solution (Buckingham, 1996)

(b) *Melting-point*: 128.4 °C (Karcher *et al.*, 1985)

(c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).

(d) *Log K<sub>ow</sub> (octanol–water)*: 6.63 (Sangster Research Laboratories, 2005)

### 14. Benzo[j]fluoranthene

#### 14.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 205-82-3

*Chem. Abstr. Name*: Benzo[j]fluoranthene

*IUPAC Systematic Name*: Benzo[j]fluoranthene

*Synonyms*: 7,8-Benzofluoranthene; 10,11-benzofluoranthene<sup>\*</sup>; benzo-12,13-fluoranthene<sup>\*</sup>; dibenzo[*ajk*]fluorene

<sup>\*</sup>Alternative numbering convention

#### 14.2 Chemical and physical properties of the pure substance

(a) *Description*: Yellow plates from alcohol; needles from acetic acid (Lide, 2005)

(b) *Melting-point*: 165.4 (Karcher *et al.*, 1985); 166 °C (Lide, 2005)

(c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).

(d) *Water solubility*: 0.0025 mg/L (Howard & Meylan, 1997)

**15. Benzo[*k*]fluoranthene**15.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 207-08-9

*Chem. Abstr. Name:* Benzo[*k*]fluoranthene

*IUPAC Systematic Name:* Benzo[*k*]fluoranthene

*Synonyms:* 8,9-Benzfluoranthene; 8,9-benzofluoranthene; 11,12-benzofluoranthene\*;  
2,3,1',8'-binaphthylene; dibenzo[*b,jk*]fluorene

\*Alternative numbering convention

15.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Pale yellow needles from benzene (Lide, 2005)
- (b) *Boiling-point:* 480 °C (Lide, 2005)
- (c) *Melting-point:* 215.7 °C (Karcher *et al.*, 1985); 217 °C (Lide, 2005)
- (d) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (e) *Water solubility:* 0.0008 mg/L at 25 °C (Pearlman *et al.*, 1984)
- (f) *Log  $K_{ow}$  (octanol–water):* 6.11 (Sangster Research Laboratories, 2005)
- (g) *Henry's law constant:* 0.044 Pa m<sup>3</sup>/mol at 20 °C (ten Hulscher *et al.*, 1992)

**16. Benzo[*a*]fluorene**16.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 238-84-6

*Chem. Abstr. Name:* 11H-Benzo[*a*]fluorene

*IUPAC Systematic Name:* 11H-Benzo[*a*]fluorene

*Synonyms:* 1,2-Benzofluorene; chrysofluorene

16.2 *Chemical and physical properties of the pure substance*

From Lide (2005), unless otherwise specified

- (a) *Description:* Plates from acetone or acetic acid
- (b) *Boiling-point:* 413 °C
- (c) *Melting-point:* 189–190 °C
- (d) *Spectroscopy data:* UV/VIS, infrared and mass spectral data have been reported (NIST, 1998, 2005).
- (e) *Water solubility:* 0.045 mg/L at 25 °C (Miller *et al.*, 1985)
- (f) *Log  $K_{ow}$  (octanol–water):* 5.40 (Sangster Research Laboratories, 2005)
- (g) *Henry's law constant:* 2.70 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)



**17. Benzo[*b*]fluorene**17.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 243-17-4

*Chem. Abstr. Name:* 11H-Benzo[*b*]fluorene

*IUPAC Systematic Name:* 11H-Benzo[*b*]fluorene

*Synonym:* 2,3-Benzofluorene

17.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Crystals from petroleum ether or acetic acid (Buckingham, 1996)
- (b) *Boiling-point:* 401–402 °C (Buckingham, 1996)
- (c) *Melting-point:* 208–209 °C (Buckingham, 1996); 213.5 °C (Karcher *et al.*, 1988); 212 °C (Lide, 2005)
- (d) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).
- (e) *Water solubility:* 0.002 mg/L at 25 °C (Pearlman *et al.*, 1984; Miller *et al.*, 1985)
- (f) *Log K<sub>ow</sub> (octanol–water):* 5.75 (Sangster Research Laboratories, 2005)

**18. Benzo[*c*]fluorene**18.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 205-12-9

*Chem. Abstr. Name:* 7H-Benzo[*c*]fluorene

*IUPAC Systematic Name:* 7H-Benzo[*c*]fluorene

*Synonym:* 3,4-Benzofluorene

18.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Plates recrystallized from ethanol (Buckingham, 1996)
- (b) *Melting-point:* 130–131 °C (Buckingham, 1996); 126.5 °C (Karcher *et al.*, 1988)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).

**19. Benzo[*ghi*]perylene**19.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 191-24-2

*Chem. Abstr. Name:* Benzo[*ghi*]perylene

*IUPAC Systematic Name:* Benzo[ghi]perylene

*Synonyms:* 1,12-Benzoperylene; 1,12-benzperylene

### 19.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Large, pale yellow-green plates from xylene (Clar, 1964)
- (b) *Melting-point:* 278.3 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility:* 0.00026 mg/L at 25 °C (Miller *et al.*, 1985)
- (e) *Log K<sub>ow</sub> (octanol–water):* 6.90 (Sangster Research Laboratories, 2005)
- (f) *Henry's law constant:* 0.027 Pa m<sup>3</sup>/mol at 20 °C (ten Hulscher *et al.*, 1992)

## 20. **Benzo[c]phenanthrene**

### 20.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 195-19-7

*Chem. Abstr. Name:* Benzo[c]phenanthrene

*IUPAC Systematic Name:* Benzo[c]phenanthrene

*Synonyms:* 3,4-Benzophenanthrene; tetrahelicene

### 20.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description:* Needles from alcohol
- (b) *Melting-point:* 68 °C; 66.1 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998)

## 21. **Benzo[a]pyrene**

### 21.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 50-32-8

*Chem. Abstr. Name:* Benzo[a]pyrene

*IUPAC Systematic Name:* Benzo[a]pyrene

*Synonyms:* BaP; benzo[def]chrysene; benz[a]pyrene; 3,4-benz[a]pyrene<sup>\*</sup>; 3,4-benzopyrene<sup>\*</sup>; 6,7-benzopyrene<sup>\*</sup>; 3,4-benzpyrene<sup>\*</sup>; 4,5-benzpyrene<sup>\*</sup>

<sup>\*</sup>Alternative numbering conventions

### 21.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Yellowish plates, needles from benzene/methanol; crystals may be monoclinic or orthorhombic
- (b) *Boiling-point*: 310–312 °C at 10 mm Hg
- (c) *Melting-point*: 179–179.3 °C; 178.1 °C (Karcher *et al.*, 1985)
- (d) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (e) *Water solubility*: 0.00162 mg/L at 25 °C (May *et al.*, 1983); 0.0038 mg/L at 25 °C (Miller *et al.*, 1985)
- (f) *Log K<sub>ow</sub> (octanol–water)*: 6.35 (Sangster Research Laboratories, 2005)
- (g) *Henry's law constant*: 0.034 Pa m<sup>3</sup>/mol at 20 °C (ten Hulscher *et al.*, 1992)

## 22. Benzo[e]pyrene

### 22.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 192-97-2

*Chem. Abstr. Name*: Benzo[e]pyrene

*IUPAC Systematic Name*: Benzo[e]pyrene

*Synonyms*: 1,2-Benzopyrene\* ; 4,5-benzopyrene; 1,2-benzpyrene\* ; 4,5-benzpyrene

\*Alternative numbering convention

### 22.2 Chemical and physical properties of the pure substance

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Prisms or plates from benzene
- (b) *Melting-point*: 178–179 °C; 178.7 (Karcher *et al.*, 1985)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility*: 0.0063 mg/L at 25 °C (Pearlman *et al.*, 1984)
- (e) *Log K<sub>ow</sub> (octanol–water)*: 6.44 (Sangster Research Laboratories, 2005)

## 23. Chrysene

### 23.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 218-01-9

*Chem. Abstr. Name*: Chrysene

*IUPAC Systematic Name*: Chrysene

*Synonyms*: Benzo[a]phenanthrene; 1,2-benzophenanthrene; 1,2-benzphenanthrene

### 23.2 Chemical and physical properties of the pure substance

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Orthorhombic bipyramidal plates from benzene
- (b) *Boiling-point*: 448 °C
- (c) *Melting-point*: 254°C; 253.8 °C (Karcher *et al.*, 1985)
- (d) *Density*: 1.274 at 20 °C relative to water at 4 °C
- (e) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (f) *Water solubility*: 0.00179 mg/L at 25 °C (May *et al.*, 1983); 0.0020 mg/L at 25 °C (Miller *et al.*, 1985)
- (g) *Log K<sub>ow</sub> (octanol–water)*: 5.79 (Miller *et al.*, 1985); 5.86 (Sangster Research Laboratories, 2005)
- (h) *Henry's law constant*: 0.53 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)

## 24. Coronene

### 24.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 191-07-1

*Chem. Abstr. Name*: Coronene

*IUPAC Systematic Name*: Coronene

*Synonyms*: Dibenzo[ghi,pqr]perylene; hexabenzobenzene

### 24.2 Chemical and physical properties of the pure substance

From Lide (2005), unless otherwise specified

- (a) *Description*: Yellow needles from benzene
- (b) *Boiling-point*: 525 °C
- (c) *Melting-point*: 437.4 °C; 439 °C (Karcher *et al.*, 1988)
- (d) *Density*: 1.371 at 25 °C
- (e) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).
- (f) *Water solubility*: 0.00014 mg/L at 25 °C (Miller *et al.*, 1985)
- (g) *Log K<sub>ow</sub> (octanol–water)*: 6.50 (Sangster Research Laboratories, 2005)

## 25. 4H-Cyclopenta[def]chrysene

### 25.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 202-98-2

*Chem. Abstr. Name*: 4H-Cyclopenta[def]chrysene

*IUPAC Systematic Name*: 4H-Cyclopenta[def]chrysene

*Synonyms*: 4,5-Methanochrysene; 4,5-methylenechrysene

## 25.2 *Chemical and physical properties of the pure substance*

- (a) *Melting-point*: 171–173 °C (Nagel *et al.*, 1977); 172.5–173.5 (Harvey *et al.*, 1991)
- (b) *Spectroscopy data*: UV/VIS, infrared and NMR spectral data have been reported (Harvey *et al.*, 1991).

## 26. **Cyclopenta[*cd*]pyrene**

### 26.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 27208-37-3

*Chem. Abstr. Name*: Cyclopenta[*cd*]pyrene

*IUPAC Systematic Name*: Cyclopenta[*cd*]pyrene

*Synonyms*: Acepyrene; acepyrylene; cyclopenta[*c,d*]pyrene

### 26.2 *Chemical and physical properties of the pure substance*

- (a) *Melting-point*: 170 °C (Karcher *et al.*, 1985)
- (b) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).

## 27. **5,6-Cyclopenteno-1,2-benzanthracene**

### 27.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 7099-43-6

*Chem. Abstr. Name*: 1H-Benzo[*a*]cyclopent[*h*]anthracene, 2,3-dihydro-

*IUPAC Systematic Name*: 2,3-Dihydro-1H-benzo[*a*]cyclopent[*h*]anthracene

*Synonym*: 5,6-Cyclopenteno-1,2-benzanthracene

### 27.2 *Chemical and physical properties of the pure substance*

- (a) *Melting-point*: 197–199 °C (Cooke, 1932)
- (b) *Spectroscopy data*: UV/VIS spectral data have been reported (Mayneord & Roe, 1935).

## 28. **Dibenz[*a,c*]anthracene**

### 28.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 215-58-7

*Chem. Abstr. Name*: Benzo[*b*]triphenylene

*IUPAC Systematic Name*: Benzo[*b*]triphenylene

*Synonyms:* 2,3-Benzotriphenylene; 1,2:3,4-dibenzanthracene; dibenzo[*a,c*]anthracene; 1,2:3,4-dibenzoanthracene

## 28.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Needles from acetic acid or alcohol (Lide, 2005)
- (b) *Melting-point:* 205 °C (Lide, 2005); 205.6 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility:* 0.0016 mg/L at 25 °C (Howard & Meyland, 1997)
- (e) *Log K<sub>ow</sub> (octanol–water):* 6.17 (Sangster Research Laboratories, 2005)

## 29. **Dibenz[*a,h*]anthracene**

### 29.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 53-70-3

*Chem. Abstr. Name:* Dibenz[*a,h*]anthracene

*IUPAC Systematic Name:* Dibenz[*a,h*]anthracene

*Synonyms:* 1,2:5,6-Benzanthracene; 1,2:5,6-dibenz[*a*]anthracene; 1,2:5,6-dibenzanthracene; dibenzo[*a,h*]anthracene; 1,2:5,6-dibenzoanthracene

### 29.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description:* Plates or leaflets from acetic acid; crystals may be monoclinic or orthorhombic
- (b) *Melting-point:* 266 °C; 266.6 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility:* 0.00050 mg/L at 25 °C (Miller *et al.*, 1985)
- (e) *Log K<sub>ow</sub> (octanol–water):* 6.75 (Sangster Research Laboratories, 2005)

## 30. **Dibenz[*a,j*]anthracene**

### 30.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 224-41-9

*Chem. Abstr. Name:* Dibenz[*a,j*]anthracene

*IUPAC Systematic Name:* Dibenz[*a,j*]anthracene

*Synonyms:* 1,2:7,8-Dibenzanthracene; 3,4:5,6-dibenzanthracene; dibenzo-1,2,7,8-anthracene

### 30.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Orange leaves or needles from benzene (Lide, 2005)
- (b) *Melting-point*: 197.3 °C (Karcher *et al.*, 1985); 197.5 °C (Lide, 2005)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility*: 0.012 mg/L at 25 °C (Pearlman *et al.*, 1984)
- (e) *Log K<sub>ow</sub> (octanol–water)*: 7.11 (Sangster Research Laboratories, 2005)

## 31. **Dibenzo[a,e]fluoranthene**

### 31.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 5385-75-1

*Chem. Abstr. Name*: Dibenz[a,e]aceanthrylene

*IUPAC Systematic Name*: Dibenz[a,e]aceanthrylene

*Synonym*: 2,3,5,6-Dibenzofluoranthene

### 31.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Yellow needles (recrystallized from benzene) (Buckingham, 1996)
- (b) *Melting-point*: 232 °C (Buckingham, 1996); 232 °C (Karcher *et al.*, 1988)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).

## 32. **13H-Dibenzo[a,g]fluorene**

### 32.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 207-83-0

*Chem. Abstr. Name*: 13H-Dibenzo[a,g]fluorene

*IUPAC Systematic Name*: 13H-Dibenzo[a,g]fluorene

*Synonyms*: Dibenzo[a,g]fluorene; 1,2,5,6-dibenzofluorene

### 32.2 *Chemical and physical properties of the pure substance*

- (a) *Melting-point*: 176–178 °C (Hopkinson *et al.*, 1986); 175–175.5 °C (Harvey *et al.*, 1991)
- (b) *Spectroscopy data*: UV/VIS and NMR spectral data have been reported (Hopkinson *et al.*, 1986; Harvey *et al.*, 1991).

**33. Dibenzo[*h,rst*]pentaphene**33.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 192-47-2

*Chem. Abstr. Name:* Dibenzo[*h,rst*]pentaphene

*IUPAC Systematic Name:* Dibenzo[*h,rst*]pentaphene

*Synonyms:* Tribenzo[*a,e,i*]pyrene; 1,2:4,5:7,8-tribenzopyrene

33.2 *Chemical and physical properties of the pure substance*

(a) *Melting-point:* 315 °C (Blümer et al., 1976)

(b) *Spectroscopy data:* Infrared and mass spectral data have been reported (NIST, 1998, 2005).

**34. Dibenzo[*a,e*]pyrene**34.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 192-65-4

*Chem. Abstr. Name:* Naphtho[1,2,3,4-*def*]chrysene

*IUPAC Systematic Name:* Naphtho[1,2,3,4-*def*]chrysene

*Synonym:* 1,2:4,5-Dibenzopyrene

34.2 *Chemical and physical properties of the pure substance*

(a) *Description:* Pale yellow needles from xylene (Lide, 2005)

(b) *Melting-point:* 244.4 °C (Karcher et al., 1985); 233.5 °C (Lide, 2005)

(c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher et al., 1985; NIST, 1998).

**35. Dibenzo[*a,h*]pyrene**35.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 189-64-0

*Chem. Abstr. Name:* Dibenzo[*b,def*]chrysene

*IUPAC Systematic Name:* Dibenzo[*b,def*]chrysene

*Synonym:* 3,4:8,9-Dibenzopyrene\*

\*Alternative numbering convention



35.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Golden-yellow plates, recrystallized from xylene or trichlorobenzene (Lide, 2005)
- (b) *Melting-point*: 317 °C (Karcher *et al.*, 1988); 315 °C (Lide, 2005)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).

**36. Dibenzo[*a,i*]pyrene**36.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 189-55-9

*Chem. Abstr. Name*: Benzo[*rst*]pentaphene

*IUPAC Systematic Name*: Benzo[*rst*]pentaphene

*Synonyms*: Benzo[*rst*]pentacene; dibenzo[*b,h*]pyrene; 1,2:7,8-dibenzpyrene

36.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Greenish yellow needles, prisms or lamellae (IARC, 1983)
- (b) *Melting-point*: 282 °C (Karcher *et al.*, 1988); 281.5 °C (Lide, 2005)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).

**37. Dibenzo[*a,l*]pyrene**37.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 191-30-0

*Chem. Abstr. Name*: Dibenzo[*def,p*]chrysene

*IUPAC Systematic Name*: Dibenzo[*def,p*]chrysene

*Synonym*: 1,2,9,10-Dibenzopyrene

37.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Yellow plates, from ethanol–benzene (Lide, 2005)
- (b) *Melting-point*: 162.4 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; 1988; NIST, 1998).
- (d) *Log K<sub>ow</sub> (octanol–water)*: 7.71 (Sangster Research Laboratories, 2005)

**38. Dibenzo[e,l]pyrene**38.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 192-51-8

*Chem. Abstr. Name:* Dibenzo[fg,op]naphthacene

*IUPAC Systematic Name:* Dibenzo[fg,op]naphthacene

*Synonyms:* 4,5,9,10-Dibenzopyrene; dibenzotetracene

38.2 *Chemical and physical properties of the pure substance*

- (a) *Spectroscopy data:* UV/VIS (Yu & Campiglia, 2004), infrared (Weisman *et al.*, 2005), phosphorescence (Schmidt *et al.*, 1987) and mass (NIST, 1998) spectral data have been reported.

**39. 1,2-Dihydroaceanthrylene**39.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 641-48-5

*Chem. Abstr. Name:* Aceanthrylene, 1,2-dihydro-

*IUPAC Systematic Name:* 1,2-Dihydroaceanthrylene

*Synonym:* Aceanthrene

39.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Yellow, flaky crystals (Becker *et al.*, 1985); colourless solid (Otero-Lobato *et al.*, 2005)
- (b) *Melting-point:* 118–119 °C (Becker *et al.*, 1985); 112–113 °C (Olde Boerrigter *et al.*, 1989; Otero-Lobato *et al.*, 2005)
- (c) *Spectroscopy data:* Proton and carbon-13 NMR and mass spectral data have been reported (Becker *et al.*, 1985; Olde Boerrigter *et al.*, 1989; Otero-Lobato *et al.*, 2005).

**40. 1,4-Dimethylphenanthrene**40.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 22349-59-3

*Chem. Abstr. Name:* Phenanthrene, 1,4-dimethyl-

*IUPAC Systematic Name:* 1,4-Dimethylphenanthrene

## 40.2 *Chemical and physical properties of the pure substance*

- (a) *Description*: Long, white needles recrystallized from methanol (Papa *et al.*, 1938); colourless needles from petroleum ether (Jung & Koreeda, 1989)
- (b) *Melting-point*: 49.5–50.5 °C (Papa *et al.*, 1938); 50–51 °C (Jung & Koreeda, 1989)
- (c) *Spectroscopy data*: Infrared, and proton and carbon-13 NMR spectral data have been reported (Jung & Koreeda, 1989).

## 41. Fluoranthene

### 41.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 206-44-0

*Chem. Abstr. Name*: Fluoranthene

*IUPAC Systematic Name*: Fluoranthene

*Synonyms*: 1,2-Benzacephthalene; 1,2-benzoacenaphthylene; benzo[*jk*]fluorene; 1,2-idryl; 1,2-(1,8-naphthalenediyl)benzene

### 41.2 *Chemical and physical properties of the pure substance*

From Lide (2005), unless otherwise specified

- (a) *Description*: Pale yellow needles or plates from alcohol
- (b) *Boiling-point*: 384 °C
- (c) *Melting-point*: 110.19 °C; 108.8 °C (Karcher *et al.*, 1985)
- (d) *Density*: 1.252 at 0 °C relative to water at 4 °C
- (e) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (f) *Water solubility*: 0.205 mg/L at 25 °C (May *et al.*, 1983); 0.26 mg/L at 25 °C (Miller *et al.*, 1985)
- (g) *Vapour pressure*: 0.00123 Pa at 25 °C (Sonnefeld *et al.*, 1983)
- (h) *Log  $K_{ow}$  (octanol–water)*: 5.20 (Sangster Research Laboratories, 2005)
- (i) *Henry's law constant*: 1.96 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)
- (j) *Atmospheric OH rate constant*:  $\sim 1.8 \times 10^{-11}$  cm<sup>3</sup>/mol/s at 100 °C (Calvert *et al.*, 2002)

## 42. Fluorene

### 42.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 86-73-7

*Chem. Abstr. Name*: 9H-Fluorene

*IUPAC Systematic Name*: 9H-Fluorene

*Synonyms:* *ortho*-Biphenylenemethane; diphenylenemethane; methane, diphenylene-; 2,2'-methylenebiphenyl

#### 42.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description:* White leaflets or flakes from alcohol
- (b) *Boiling-point:* 295 °C
- (c) *Melting-point:* 116–117 °C; 115–116 °C (Karcher *et al.*, 1988)
- (d) *Density:* 1.20
- (e) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).
- (f) *Water solubility:* 1.68 mg/L at 25 °C (May *et al.*, 1983)
- (g) *Vapour pressure:* 0.08 Pa at 25 °C (Sonnefeld *et al.*, 1983)
- (h) *Log K<sub>ow</sub> (octanol–water):* 4.18 (Miller *et al.*, 1985); 4.18 (Sangster Research Laboratories, 2005)
- (i) *Henry's law constant:* 9.81 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)
- (j) *Atmospheric OH rate constant:* 1.4 × 10<sup>-11</sup> cm<sup>3</sup>/mol/s at 25 °C (Calvert *et al.*, 2002)

### 43. **Indeno[1,2,3-cd]pyrene**

#### 43.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 193-39-5

*Chem. Abstr. Name:* Indeno[1,2,3-cd]pyrene

*IUPAC Systematic Name:* Indeno[1,2,3-cd]pyrene

*Synonyms:* 1,10-(*ortho*-Phenylene)pyrene; 1,10-(1,2-phenylene)pyrene

#### 43.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Yellow plates or needles (recrystallized from light petroleum solution) showing a greenish yellow fluorescence; yellow crystals from cyclohexane (IARC, 1983; Lide, 2005)
- (b) *Melting-point:* 163.6 °C (Karcher *et al.*, 1985)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility:* 0.00019 mg/L at 25 °C (Pearlman *et al.*, 1984)
- (e) *Henry's law constant:* 0.029 Pa m<sup>3</sup>/mol at 20 °C (ten Hulscher *et al.*, 1992)

**44. 1-Methylchrysene**44.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 3351-28-8

*Chem. Abstr. Name:* Chrysene, 1-methyl-

*IUPAC Systematic Name:* 1-Methylchrysene

44.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Leaflets recrystallized from benzene, hexane or toluene (Lide, 1992)
- (b) *Melting-point:* 254.4 °C (Karcher *et al.*, 1985); 256–257 °C (Lide, 1992)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).

**45. 2-Methylchrysene**45.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 3351-32-4

*Chem. Abstr. Name:* Chrysene, 2-methyl-

*IUPAC Systematic Name:* 2-Methylchrysene

45.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Leaflets recrystallized from benzene–alcohol (Lide, 1992)
- (b) *Melting-point:* 230.2 °C (Karcher *et al.*, 1985); 229–230 °C (Lide, 1992)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).

**46. 3-Methylchrysene**46.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 3351-31-3

*Chem. Abstr. Name:* Chrysene, 3-methyl-

*IUPAC Systematic Name:* 3-Methylchrysene

46.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Leaflets recrystallized from benzene–petroleum ether (Lide, 2005)
- (b) *Melting-point:* 171.9 °C (Karcher *et al.*, 1985); 173.3 °C (Lide, 2005)

- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).

#### 47. 4-Methylchrysene

##### 47.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 3351-30-2

*Chem. Abstr. Name*: Chrysene, 4-methyl-

*IUPAC Systematic Name*: 4-Methylchrysene

##### 47.2 Chemical and physical properties of the pure substance

- (a) *Description*: Highly fluorescent plates recrystallized from benzene–ethanol (Buckingham, 1996)
- (b) *Melting-point*: 150.6 °C (Karcher *et al.*, 1985); 151–152 °C (Buckingham, 1996)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported spectra (Karcher *et al.*, 1985; NIST, 1998).

#### 48. 5-Methylchrysene

##### 48.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 3697-24-3

*Chem. Abstr. Name*: Chrysene, 5-methyl-

*IUPAC Systematic Name*: 5-Methylchrysene

##### 48.2 Chemical and physical properties of the pure substance

- (a) *Description*: Needles recrystallized from benzene–ethanol with a brilliant bluish violet fluorescence in UV light (Buckingham, 1996)
- (b) *Melting-point*: 117.1 °C (Karcher *et al.*, 1985); 118–119 °C (Buckingham, 1996)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility*: 0.062 mg/L at 27 °C (Howard & Meylan, 1997)

#### 49. 6-Methylchrysene

##### 49.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 1705-85-7

*Chem. Abstr. Name*: Chrysene, 6-methyl-

*IUPAC Systematic Name:* 6-Methylchrysene

49.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Fluorescent needles recrystallized from ethyl acetate–ethanol (Buckingham, 1996)
- (b) *Melting-point:* 160–161 °C (Karcher *et al.*, 1985); 161–162 °C (Buckingham, 1996)
- (c) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (d) *Water solubility:* 0.065 mg/L at 27 °C (Howard & Meylan, 1997)

**50. 2-Methylfluoranthene**

50.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 33543-31-6

*Chem. Abstr. Name:* Fluoranthene, 2-methyl-

*IUPAC Systematic Name:* 2-Methylfluoranthene

Note: Previously 3-methylfluoranthene

50.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Ill-defined needles after crystallization from methanol (Tucker, 1952)
- (b) *Melting-point:* 79–81 °C (Tucker, 1952)
- (c) *Spectroscopy data:* Mass spectral data have been reported (NIST, 1998).

**51. 3-Methylfluoranthene**

51.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 1706-01-0

*Chem. Abstr. Name:* Fluoranthene, 3-methyl-

*IUPAC Systematic Name:* 3-Methylfluoranthene

Note: Previously 4-methylfluoranthene

51.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Pale green sword blades recrystallized from ethanol (Stubbs & Tucker, 1950)
- (b) *Melting-point:* 65–66 °C (Stubbs & Tucker, 1950); 66–68 °C (Karcher *et al.*, 1991)

- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1991).

## 52. 1-Methylphenanthrene

### 52.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 832-69-9

*Chem. Abstr. Name*: Phenanthrene, 1-methyl-

*IUPAC Systematic Name*: 1-Methylphenanthrene

### 52.2 Chemical and physical properties of the pure substance

- (a) *Description*: Leaves or plates recrystallized from diluted alcohol (Lide, 2005)
- (b) *Melting-point*: 123 °C (Lide, 2005; Karcher *et al.*, 1991)
- (c) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1991; NIST, 1998).
- (d) *Water solubility*: 0.269 mg/L at 25 °C (May *et al.*, 1983)
- (e) *Log K<sub>ow</sub> (octanol–water)*: 5.08 (Sangster Research Laboratories, 2005)
- (f) *Henry's law constant*: 5.00 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)
- (g) *Atmospheric OH rate constant*: 2.88 × 10<sup>-11</sup> cm<sup>3</sup>/mol/s at 25 °C (Lee *et al.*, 2003)

## 53. Naphtho[1,2-*b*]fluoranthene

### 53.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 111189-32-3

*Chem. Abstr. Name*: Indeno[1,2,3-*hi*]chrysene

*IUPAC Systematic Name*: Indeno[1,2,3-*hi*]chrysene

### 53.2 Chemical and physical properties of the pure substance

- (a) *Description*: Long greenish yellow needles from ethyl acetate/hexane (Cho & Harvey, 1987a)
- (b) *Melting-point*: 188–189 °C (Cho & Harvey, 1987a)
- (c) *Spectroscopy data*: UV/VIS, and proton and carbon-13 NMR spectral data have been reported (Cho & Harvey, 1987a,b).

## 54. Naphtho[2,1-*a*]fluoranthene

### 54.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 203-20-3



*Chem. Abstr. Name:* Dibenz[*a,j*]aceanthrylene  
*IUPAC Systematic Name:* Dibenz[*a,j*]aceanthrylene  
*Synonym:* 15,16-Benzodehydrocholanthrene

54.2 *Chemical and physical properties of the pure substance*

- (a) *Description:* Bright yellow, cottony needles recrystallized from benzene (Fieser & Seligman, 1935)
- (b) *Melting-point:* 181–181.3 °C (Fieser & Seligman, 1935); 180 °C (Ray & Harvey, 1982; Cho & Harvey, 1987a)
- (c) *Spectroscopy data:* NMR spectral data have been reported (Ray & Harvey, 1982; Cho & Harvey, 1987a).

**55. Naphtho[2,3-*e*]pyrene**

55.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 193-09-9  
*Chem. Abstr. Name:* Dibenzo[*de,qr*]naphthacene  
*IUPAC Systematic Name:* Dibenzo[*de,qr*]naphthacene  
*Synonyms:* Dibenzo[*de,qr*]tetracene; naphtho-(2',3':4,5)-pyrene

55.2 *Chemical and physical properties of the pure substance*

- (a) *Spectroscopy data:* UV/VIS and fluorescence spectral data have been reported (Schmidt *et al.*, 1987; NIST, 2005).

**56. Perylene**

56.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.:* 198-55-0  
*Chem. Abstr. Name:* Perylene  
*IUPAC Systematic Name:* Perylene  
*Synonyms:* Dibenz[*de,kl*]anthracene; *peri*-dinaphthalene;  $\alpha$ -perylene

56.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description:* Yellow to colourless crystals from toluene
- (b) *Boiling-point:* Sublimes at 350–400 °C
- (c) *Melting-point:* 273–274 °C; 277.5 °C (Karcher *et al.*, 1988)
- (d) *Density:* 1.35

- (e) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).
- (f) *Water solubility*: 0.00040 mg/L at 25 °C (Miller *et al.*, 1985)
- (g) *Vapour pressure*:  $5.85 \times 10^{-7}$  Pa at 25 °C (Howard & Meylan, 1997)
- (h) *Log  $K_{ow}$  (octanol–water)*: 6.25 (Sangster Research Laboratories, 2005)

## 57. Phenanthrene

### 57.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 85-01-8

*Chem. Abstr. Name*: Phenanthrene

*IUPAC Systematic Name*: Phenanthrene\*

*Synonym*: Phenanthrin

\*Numbering exception

### 57.2 Chemical and physical properties of the pure substance

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Monoclinic plates from alcohol
- (b) *Boiling-point*: 340 °C
- (c) *Melting-point*: 100 °C; 100.5 °C (Karcher *et al.*, 1985); 99.24 °C (Lide, 2005)
- (d) *Density*: 1.179 at 25 °C; 0.9800 relative to water at 4 °C (Lide, 2005)
- (e) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (f) *Water solubility*: 0.977 mg/L at 25 °C (May *et al.*, 1983); 1.18 mg/L at 25 °C (Miller *et al.*, 1985)
- (g) *Vapour pressure*: 0.016 Pa at 25 °C (Sonnefeld *et al.*, 1983)
- (h) *Log  $K_{ow}$  (octanol–water)*: 4.57 (Miller *et al.*, 1985); 4.52 (Sangster Research Laboratories, 2005)
- (i) *Henry's law constant*: 4.29 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)
- (j) *Atmospheric OH rate constant*:  $1.8 \times 10^{-11}$  cm<sup>3</sup>/mol/s at 25 °C (Calvert *et al.*, 2002)

## 58. Picene

### 58.1 Nomenclature

*Chem. Abstr. Services Reg. No.*: 213-46-7

*Chem. Abstr. Name*: Picene

*IUPAC Systematic Name*: Picene

*Synonyms*: Benzo[*a*]chrysene; dibenzo[*a,i*]phenanthrene; 1,2;7,8-dibenzophenanthrene

58.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Fluorescent plates from ethyl acetate
- (b) *Boiling-point*: 518–520 °C
- (c) *Melting-point*: 366–367 °C; 364 °C (Karcher *et al.*, 1988)
- (d) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).
- (e) *Water solubility*: 0.00431 mg/L at 20 °C (Howard & Meylan, 1997)
- (f) *Log K<sub>ow</sub> (octanol–water)*: 7.11 (Sangster Research Laboratories, 2005)

**59. Pyrene**59.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 129-00-0

*Chem. Abstr. Name*: Pyrene

*IUPAC Systematic Name*: Pyrene

*Synonyms*: Benzo[*def*]phenanthrene; β-pyrene

59.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description*: Monoclinic prismatic tablets from alcohol
- (b) *Boiling-point*: 404 °C
- (c) *Melting-point*: 156 °C; 150.4 °C (Karcher *et al.*, 1985); 150.6 °C (Lide, 2005)
- (d) *Density*: 1.271 at 23 °C; 1.271 at 23 °C relative to water at 4 °C (Lide, 2005)
- (e) *Spectroscopy data*: UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1985; NIST, 1998).
- (f) *Water solubility*: 0.130 mg/L at 25 °C (May *et al.*, 1983); 0.135 mg/L (Miller *et al.*, 1985)
- (g) *Vapour pressure*: 0.00060 Pa at 25 °C (Sonnefeld *et al.*, 1983)
- (h) *Log K<sub>ow</sub> (octanol–water)*: 5.18 (Miller *et al.*, 1985); 5.00 (Sangster Research Laboratories, 2005)
- (i) *Henry's law constant*: 1.71 Pa m<sup>3</sup>/mol at 25 °C (Bamford *et al.*, 1999)

**60. Triphenylene**60.1 *Nomenclature*

*Chem. Abstr. Services Reg. No.*: 217-59-4

*Chem. Abstr. Name*: Triphenylene

*IUPAC Systematic Name*: Triphenylene

*Synonyms:* Benzo[*I*]phenanthrene; 9,10-benzophenanthrene; 9,10-benzphenanthrene; 1,2,3,4-dibenznaphthalene; isochrysene

60.2 *Chemical and physical properties of the pure substance*

From O'Neil (2006), unless otherwise specified

- (a) *Description:* Long needles recrystallized from alcohol or chloroform
- (b) *Boiling-point:* 425 °C
- (c) *Melting-point:* 199 °C; 199 °C (Karcher *et al.*, 1988)
- (d) *Density:* 1.302
- (e) *Spectroscopy data:* UV/VIS, infrared, fluorescence, mass and NMR spectral data have been reported (Karcher *et al.*, 1988; NIST, 1998).
- (f) *Water solubility:* 0.00632 mg/L at 25 °C (May *et al.*, 1983)
- (g) *Log K<sub>ow</sub> (octanol–water):* 5.49 (Sangster Research Laboratories, 2005)

**Table 1. Identification of the polycyclic aromatic hydrocarbons covered in this monograph**

Common name (name used in this volume)	IUPAC name	CAS Registry No.	Molecular formula	Relative molecular mass
Acenaphthene	Acenaphthene	83-32-9	C <sub>12</sub> H <sub>10</sub>	154.2
Acepyrene	3,4-Dihydrocyclopenta[ <i>cd</i> ]pyrene	25732-74-5	C <sub>18</sub> H <sub>12</sub>	228.3
Anthanthrene	Dibenzo[ <i>def,mno</i> ]chrysene	191-26-4	C <sub>22</sub> H <sub>12</sub>	276.3
Anthracene	Anthracene	120-12-7	C <sub>14</sub> H <sub>10</sub>	178.2
11 <i>H</i> -Benz[ <i>b,c</i> ]aceanthrylene	11 <i>H</i> -Benz[ <i>b,c</i> ]aceanthrylene	202-94-8	C <sub>19</sub> H <sub>12</sub>	240.3
Benz[ <i>j</i> ]aceanthrylene	Benz[ <i>j</i> ]aceanthrylene	202-33-5	C <sub>20</sub> H <sub>12</sub>	252.3
Benz[ <i>l</i> ]aceanthrylene	Benz[ <i>l</i> ]aceanthrylene	211-91-6	C <sub>20</sub> H <sub>12</sub>	252.3
Benz[ <i>a</i> ]anthracene	Benz[ <i>a</i> ]anthracene	56-55-3	C <sub>18</sub> H <sub>12</sub>	228.3
Benzo[ <i>b</i> ]chrysene	Benzo[ <i>b</i> ]chrysene	214-17-5	C <sub>22</sub> H <sub>14</sub>	278.4
Benzo[ <i>g</i> ]chrysene	Benzo[ <i>g</i> ]chrysene	196-78-1	C <sub>22</sub> H <sub>14</sub>	278.4
Benzo[ <i>a</i> ]fluoranthene	Benzo[ <i>a</i> ]aceanthrylene	203-33-8	C <sub>20</sub> H <sub>12</sub>	252.3
Benzo[ <i>b</i> ]fluoranthene	Benz[ <i>e</i> ]acephenanthrylene	205-99-2	C <sub>20</sub> H <sub>12</sub>	252.3
Benzo[ <i>ghi</i> ]fluoranthene	Benzo[ <i>ghi</i> ]fluoranthene	203-12-3	C <sub>18</sub> H <sub>10</sub>	226.3
Benzo[ <i>j</i> ]fluoranthene	Benzo[ <i>j</i> ]fluoranthene	205-82-3	C <sub>20</sub> H <sub>12</sub>	252.3
Benzo[ <i>k</i> ]fluoranthene	Benzo[ <i>k</i> ]fluoranthene	207-08-9	C <sub>20</sub> H <sub>12</sub>	252.3
Benzo[ <i>a</i> ]fluorene	11 <i>H</i> -Benzo[ <i>a</i> ]fluorene	238-84-6	C <sub>17</sub> H <sub>12</sub>	216.3
Benzo[ <i>b</i> ]fluorene	11 <i>H</i> -Benzo[ <i>b</i> ]fluorene	243-17-4	C <sub>17</sub> H <sub>12</sub>	216.3
Benzo[ <i>c</i> ]fluorene	7 <i>H</i> -Benzo[ <i>c</i> ]fluorene	205-12-9	C <sub>17</sub> H <sub>12</sub>	216.3
Benzo[ <i>ghi</i> ]perylene	Benzo[ <i>ghi</i> ]perylene	191-24-2	C <sub>22</sub> H <sub>12</sub>	276.3
Benzo[ <i>c</i> ]phenanthrene	Benzo[ <i>c</i> ]phenanthrene	195-19-7	C <sub>18</sub> H <sub>12</sub>	228.3
Benzo[ <i>a</i> ]pyrene	Benzo[ <i>a</i> ]pyrene	50-32-8	C <sub>20</sub> H <sub>12</sub>	252.3
Benzo[ <i>e</i> ]pyrene	Benzo[ <i>e</i> ]pyrene	192-97-2	C <sub>20</sub> H <sub>12</sub>	252.3
Chrysene	Chrysene	218-01-9	C <sub>18</sub> H <sub>12</sub>	228.3
Coronene	Coronene	191-07-1	C <sub>24</sub> H <sub>12</sub>	300.4
4 <i>H</i> -Cyclopenta[ <i>def</i> ]chrysene	4 <i>H</i> -Cyclopenta[ <i>def</i> ]chrysene	202-98-2	C <sub>19</sub> H <sub>12</sub>	240.3
Cyclopenta[ <i>cd</i> ]pyrene	Cyclopenta[ <i>cd</i> ]pyrene	27208-37-3	C <sub>18</sub> H <sub>10</sub>	226.3
5,6-Cyclopenteno-1,2-benzanthracene	2,3-Dihydro-1 <i>H</i> -benzo[ <i>a</i> ]cyclopent[ <i>h</i> ]anthracene	7099-43-6	C <sub>21</sub> H <sub>16</sub>	268.4
Dibenzo[ <i>a,c</i> ]anthracene	Benzo[ <i>b</i> ]triphenylene	215-58-7	C <sub>22</sub> H <sub>14</sub>	278.4
Dibenzo[ <i>a,h</i> ]anthracene	Dibenzo[ <i>a,h</i> ]anthracene	53-70-3	C <sub>22</sub> H <sub>14</sub>	278.4

**Table 1 (Contd)**

Common name (name used in this volume)	IUPAC name	CAS Registry No.	Molecular formula	Relative molecular mass
Dibenz[ <i>a,j</i> ]anthracene	Dibenz[ <i>a,j</i> ]anthracene	224-41-9	C <sub>22</sub> H <sub>14</sub>	278.4
Dibenzo[ <i>a,e</i> ]fluoranthene	Dibenz[ <i>a,e</i> ]aceanthrylene	5385-75-1	C <sub>24</sub> H <sub>14</sub>	302.4
13 <i>H</i> -Dibenzo[ <i>a,g</i> ]fluorene	13 <i>H</i> -Dibenzo[ <i>a,g</i> ]fluorene	207-83-0	C <sub>21</sub> H <sub>14</sub>	266.3
Dibenzo[ <i>h,rst</i> ]pentaphene	Dibenzo[ <i>h,rst</i> ]pentaphene	192-47-2	C <sub>28</sub> H <sub>16</sub>	352.4
Dibenzo[ <i>a,e</i> ]pyrene	Naphtho[1,2,3,4- <i>def</i> ]chrysene	192-65-4	C <sub>24</sub> H <sub>14</sub>	302.4
Dibenzo[ <i>a,h</i> ]pyrene	Dibenzo[ <i>b,def</i> ]chrysene	189-64-0	C <sub>24</sub> H <sub>14</sub>	302.4
Dibenzo[ <i>a,i</i> ]pyrene	Benzo[ <i>rst</i> ]pentaphene	189-55-9	C <sub>24</sub> H <sub>14</sub>	302.4
Dibenzo[ <i>a,l</i> ]pyrene	Dibenzo[ <i>def,p</i> ]chrysene	191-30-0	C <sub>24</sub> H <sub>14</sub>	302.4
Dibenzo[ <i>e,l</i> ]pyrene	Dibenzo[ <i>fg,op</i> ]naphthacene	192-51-8	C <sub>24</sub> H <sub>14</sub>	302.4
1,2-Dihydroaceanthrylene	1,2-Dihydroaceanthrylene	641-48-5	C <sub>16</sub> H <sub>12</sub>	204.3
1,4-Dimethylphenanthrene	1,4-Dimethylphenanthrene	22349-59-3	C <sub>16</sub> H <sub>14</sub>	206.3
Fluoranthene	Fluoranthene	206-44-0	C <sub>16</sub> H <sub>10</sub>	202.3
Fluorene	9 <i>H</i> -Fluorene	86-73-7	C <sub>13</sub> H <sub>10</sub>	166.2
Indeno[1,2,3- <i>cd</i> ]pyrene	Indeno[1,2,3- <i>cd</i> ]pyrene	193-39-5	C <sub>22</sub> H <sub>12</sub>	276.3
1-Methylchrysene	1-Methylchrysene	3351-28-8	C <sub>19</sub> H <sub>14</sub>	242.3
2-Methylchrysene	2-Methylchrysene	3351-32-4	C <sub>19</sub> H <sub>14</sub>	242.3
3-Methylchrysene	3-Methylchrysene	3351-31-3	C <sub>19</sub> H <sub>14</sub>	242.3
4-Methylchrysene	4-Methylchrysene	3351-30-2	C <sub>19</sub> H <sub>14</sub>	242.3
5-Methylchrysene	5-Methylchrysene	3697-24-3	C <sub>19</sub> H <sub>14</sub>	242.3
6-Methylchrysene	6-Methylchrysene	1705-85-7	C <sub>19</sub> H <sub>14</sub>	242.3
2-Methylfluoranthene	2-Methylfluoranthene	33543-31-6	C <sub>17</sub> H <sub>12</sub>	216.3
3-Methylfluoranthene	3-Methylfluoranthene	1706-01-0	C <sub>17</sub> H <sub>12</sub>	216.3
1-Methylphenanthrene	1-Methylphenanthrene	832-69-9	C <sub>15</sub> H <sub>12</sub>	192.3
Naphtho[1,2- <i>b</i> ]fluoranthene	Indeno[1,2,3- <i>hi</i> ]chrysene	111189-32-3	C <sub>24</sub> H <sub>14</sub>	302.4
Naphtho[2,1- <i>a</i> ]fluoranthene	Dibenz[ <i>a,j</i> ]aceanthrylene	203-20-3	C <sub>24</sub> H <sub>14</sub>	302.4
Naphtho[2,3- <i>e</i> ]pyrene	Dibenzo[ <i>de,qr</i> ]naphthacene	193-09-9	C <sub>24</sub> H <sub>14</sub>	302.4
Perylene	Perylene	198-55-0	C <sub>20</sub> H <sub>12</sub>	252.3

**Table 1 (Contd)**

Common name (name used in this volume)	IUPAC name	CAS Registry No.	Molecular formula	Relative molecular mass
Phenanthrene	Phenanthrene	85-01-8	C <sub>14</sub> H <sub>10</sub>	178.2
Picene	Picene	213-46-7	C <sub>22</sub> H <sub>14</sub>	278.4
Pyrene	Pyrene	129-00-0	C <sub>16</sub> H <sub>10</sub>	202.3
Triphenylene	Triphenylene	217-59-4	C <sub>18</sub> H <sub>12</sub>	228.3

Compiled from IUPAC (1979), Chemical Abstract Services (1978)

**Table 2. Selected physical and chemical properties of the polycyclic aromatic compounds covered in this monograph<sup>a</sup>**

Compound	Melting-point (°C)	Vapour pressure (Pa at 25 °C)	<i>n</i> -Octanol:water partition coefficient (log $K_{ow}$ )	Solubility in water at 25 °C <sup>d</sup> (mg/L)	Henry's law constant at 25 °C (Pa•m <sup>3</sup> /mol)
Acenaphthene	95	0.29	3.92	3.9	18.5
Acepyrene	133–134	–	–	–	–
Anthanthrene	264	–	7.04	–	–
Anthracene	216.4	$8.0 \times 10^{-4}$	4.5	0.0436	5.64
11 <i>H</i> -Benz[ <i>b,c</i> ]aceanthrylene	123	–	–	–	–
Benz[ <i>j</i> ]aceanthrylene	170–171	–	–	–	–
Benz[ <i>l</i> ]aceanthrylene	157–158	–	–	–	–
Benz[ <i>a</i> ]anthracene	160.7	$2.8 \times 10^{-5}$	5.91	0.0090	1.22
Benzo[ <i>b</i> ]chrysene	294	–	7.11	–	–
Benzo[ <i>g</i> ]chrysene	116	–	–	–	–
Benzo[ <i>a</i> ]fluoranthene	146.3	–	–	–	–
Benzo[ <i>b</i> ]fluoranthene	168.3	–	5.78	0.0015	0.051
Benzo[ <i>ghi</i> ]fluoranthene	128.4	–	6.63	–	–
Benzo[ <i>j</i> ]fluoranthene	165.4	–	–	0.0025	–
Benzo[ <i>k</i> ]fluoranthene	215.7	–	6.11	0.0008	0.044
Benzo[ <i>a</i> ]fluorene	189–190	–	5.40	0.045	2.70
Benzo[ <i>b</i> ]fluorene	213.5	–	5.75	0.002	–
Benzo[ <i>c</i> ]fluorene	126.5	–	–	–	–
Benzo[ <i>ghi</i> ]perylene	278.3	–	6.90	0.00026	0.027 (20 °C)
Benzo[ <i>c</i> ]phenanthrene	66.1	–	–	–	–
Benzo[ <i>a</i> ]pyrene	178.1	–	6.35	0.00162; 0.0038	0.034
Benzo[ <i>e</i> ]pyrene	178.7	–	6.44	0.0063	–
Chrysene	253.8	–	5.86	0.00179	0.53
Coronene	439	–	6.50	0.00014	–
4 <i>H</i> -Cyclopenta[ <i>def</i> ]chrysene	171–173	–	–	–	–
Cyclopenta[ <i>cd</i> ]pyrene	170	–	–	–	–
5,6-Cyclopenteno-1,2-benzanthracene	197–199	–	–	–	–



Table 2 (Contd)

Compound	Melting-point (°C)	Vapour pressure (Pa at 25 °C)	<i>n</i> -Octanol:water partition coefficient (log $K_{ow}$ )	Solubility in water at 25 °C <sup>d</sup> (mg/L)	Henry's law constant at 25 °C (Pa•m <sup>3</sup> /mol)
Dibenz[ <i>a,c</i> ]anthracene	205.6	—	6.17	0.0016	—
Dibenz[ <i>a,h</i> ]anthracene	266.6	—	6.75	0.00050	—
Dibenz[ <i>a,j</i> ]anthracene	197.3	—	7.11	0.012	—
Dibenzo[ <i>a,e</i> ]fluoranthene	232	—	—	—	—
13 <i>H</i> -Dibenzo[ <i>a,g</i> ]fluorene	176–178	—	—	—	—
Dibenzo[ <i>h,rsi</i> ]pentaphene	315	—	—	—	—
Dibenzo[ <i>a,e</i> ]pyrene	244.4	—	—	—	—
Dibenzo[ <i>a,h</i> ]pyrene	317	—	—	—	—
Dibenzo[ <i>a,i</i> ]pyrene	282	—	—	—	—
Dibenzo[ <i>a,l</i> ]pyrene	162.4	—	7.71	—	—
Dibenzo[ <i>e,l</i> ]pyrene	—	—	—	—	—
1,2-Dihydroaceanthrylene	118–119	—	—	—	—
1,4-Dimethylphenanthrene	50–51	—	—	—	—
Fluoranthene	108.8	0.00123	5.20	0.205; 0.26	1.96
Fluorene	115–116	0.08	4.18	1.68	9.81
Indeno[1,2,3- <i>cd</i> ]pyrene	163.6	—	—	0.00019	0.029 (20 °C)
1-Methylchrysene	254.4	—	—	—	—
2-Methylchrysene	230.2	—	—	—	—
3-Methylchrysene	171.9	—	—	—	—
4-Methylchrysene	150.6	—	—	—	—
5-Methylchrysene	117.1	—	—	0.062 (27 °C)	—
6-Methylchrysene	160–161	—	—	0.065 (27 °C)	—
2-Methylfluoranthene	79–81	—	—	—	—
3-Methylfluoranthene	65–66	—	—	—	—
1-Methylphenanthrene	123	—	5.08	0.269	5.00
Naphtho[1,2- <i>b</i> ]fluoranthene	188–189	—	—	—	—

**Table 2 (Contd)**

Compound	Melting-point (°C)	Vapour pressure (Pa at 25 °C)	<i>n</i> -Octanol:water partition coefficient (log $K_{ow}$ )	Solubility in water at 25 °C <sup>d</sup> (mg/L)	Henry's law constant at 25 °C (Pa•m <sup>3</sup> /mol)
Naphtho[2,1- <i>a</i> ]fluoranthene	180	–	–	–	–
Naphtho[2,3- <i>e</i> ]pyrene	–	–	–	–	–
Perylene	277.5	–	6.25	0.0004	–
Phenanthrene	100.5	0.016	4.52	0.977; 1.18	4.29
Picene	364	–	7.11	0.00431	–
Pyrene	150.4	0.00060	5.00	0.130; 0.135	1.71
Triphenylene	199	–	5.49	0.00632	–

<sup>a</sup> For the original references that contain measurement details, refer to the text.

–, not available

**Figure 1. Structural formulae of polycyclic aromatic hydrocarbons covered in this monograph**

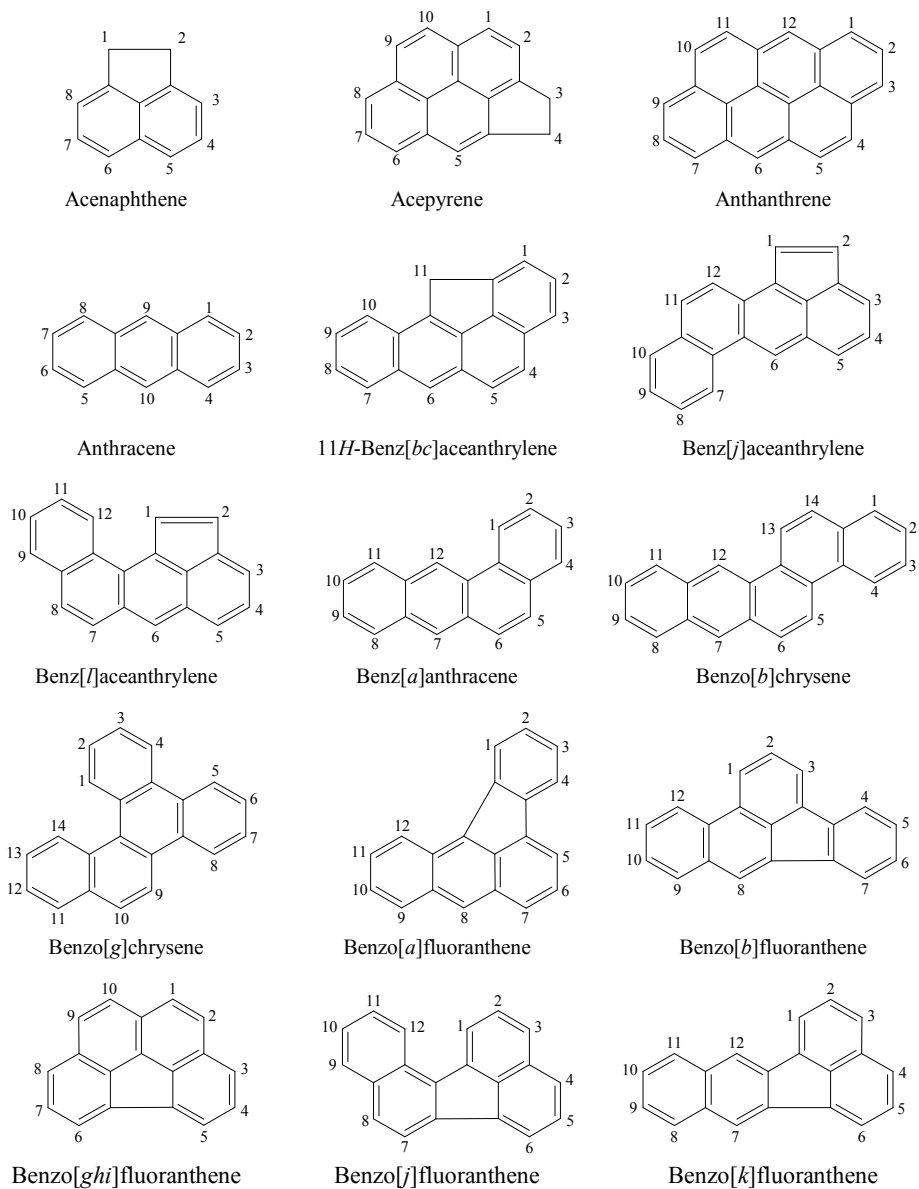
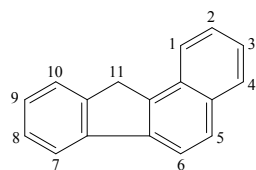
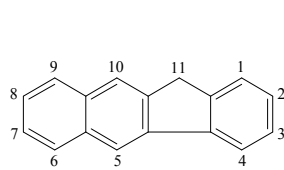


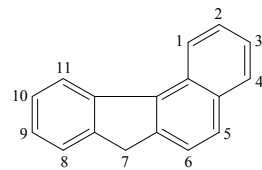
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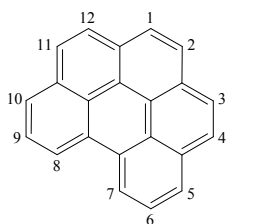
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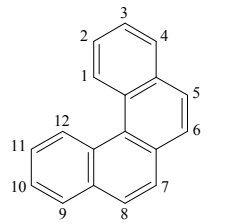
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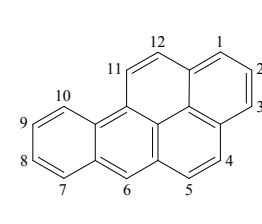
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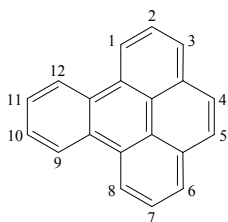
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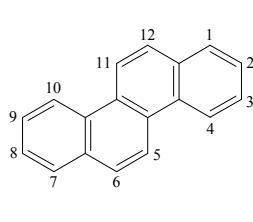
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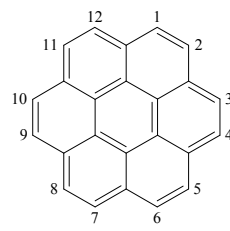
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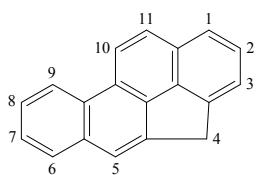
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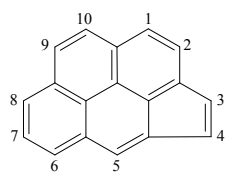
Chrysene



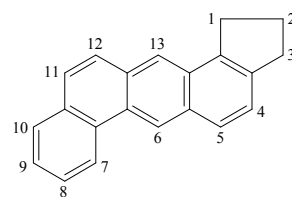
Coronene



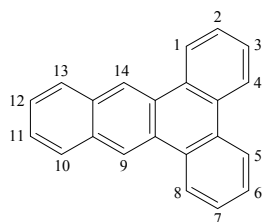
4H-Cyclopenta[def]chrysene



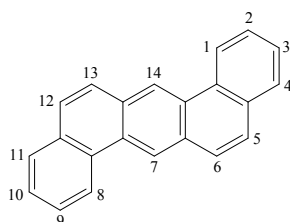
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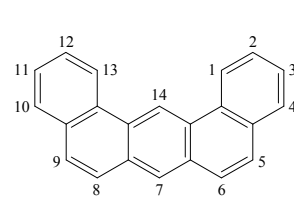
5,6-Cyclopenteno-1,2-benzanthracene



Dibenz[a,c]anthracene



Dibenz[a,h]anthracene



Dibenz[a,j]anthracene

Figure 1 (contd)

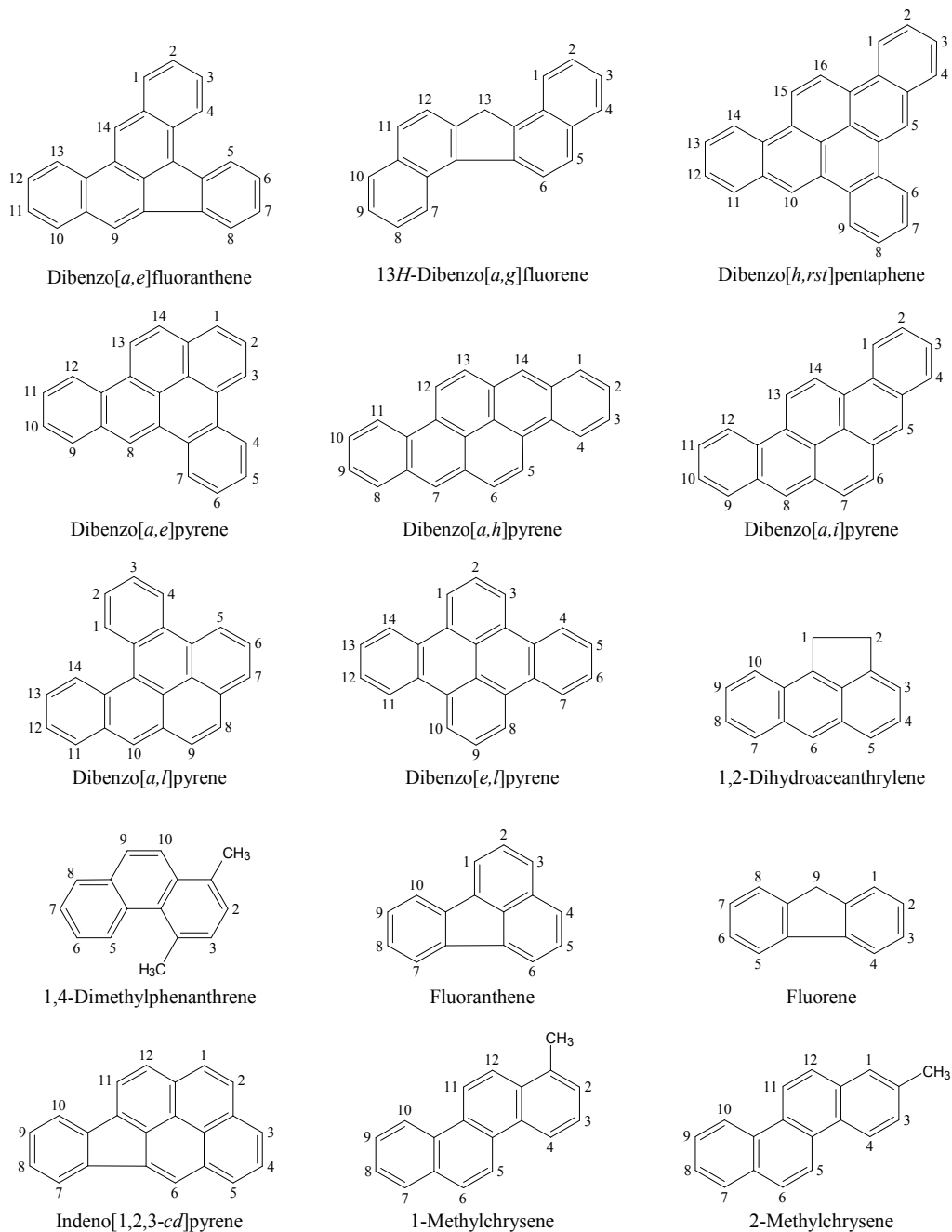
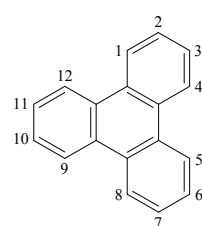
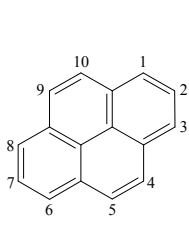
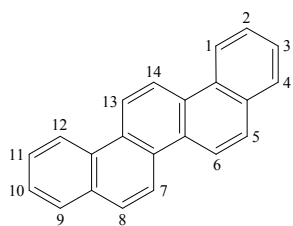
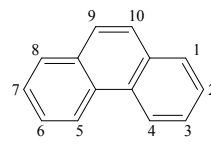
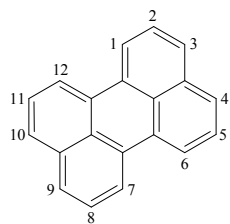
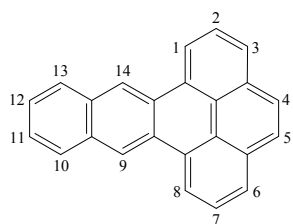
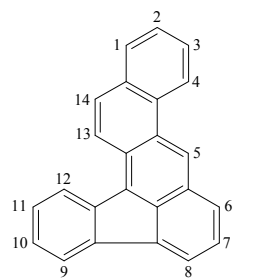
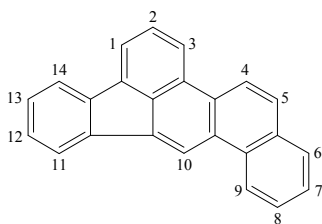
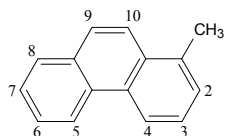
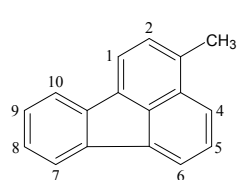
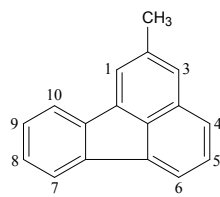
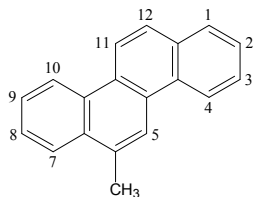
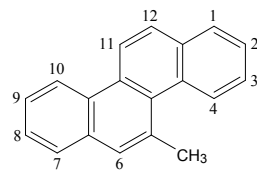
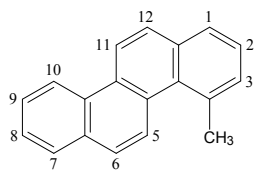
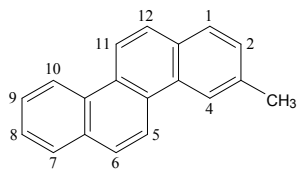


Figure 1 (contd)



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