

Supporting Information

Advances in Pretreatment and Analysis Methods of Aromatic Hydrocarbons in Soil

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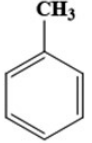
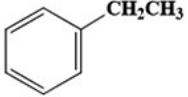
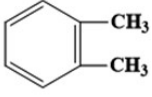

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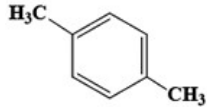
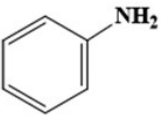
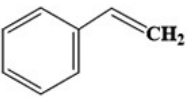
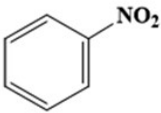
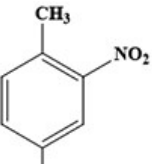
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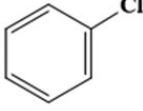
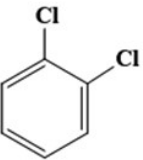
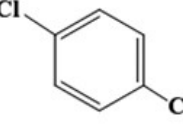
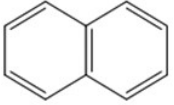
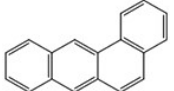
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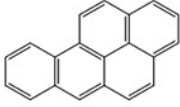
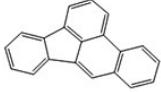
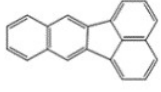
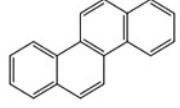
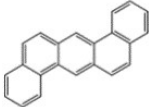
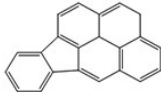
Supporting Table

Table S-1. Physicochemical properties, toxicity and the pollution risk guidance values of common monocyclic aromatic hydrocarbons and their ramification and PAHs in soil.

| NO. | Chemical Name Abbreviation | Chemical Structure | Physical Description | Physicochemical Properties | Pollution Risk Guidance Values(mg/kg) | | Toxicity |
|--|-------------------------------|---|---|--|---------------------------------------|-----------------|--|
| | | | | | Residential Land | Industrial Land | |
| A) Monocyclic aromatic hydrocarbons and derivatives | | | | | | | |
| 1 | Benzene |  | Achromaticity and clarity Volatile liquid Aromatic odor | (1) BP: 80 °C (2) MP: 5.5 °C (3) 1.7 g/1L Water; Soluble in alcohol, ether, acetone, chloroform, gasoline and other organic solvents (4) LogP: 2.03 | 0.064 | 0.26 | Carcinogen: Group 1 LD50: Rat transoral 3306 mg/kg Mouse transdermal 48 mg/kg |
| 2 | Toluene |  | Colorless transparent Liquid Aromatic odor | (1) BP: 110.6 °C (2) MP: -95 °C (3) 0.52 g/1L Water; Miscible in benzene, alcohol, ether and other organic solvents (4) LogP: 2.52 | 120 | 672 | Carcinogen: Group 3 LD50: Rat transoral 5000 mg/kg 71.4 g/m3 human inhalation, short term lethal |
| 3 | Ethybenzene |  | Colorless oily liquid Aromatic odor | (1) BP: 136.2 °C (2) MP: -94 °C (3) 0.16 g/1L Water; Miscible in benzene, alcohol, ether and other organic solvents (4) LogP: 3.17 | 0.2 | 0.81 | Carcinogen: Group 2A LD50: Rat transoral 3500 mg/kg Rabbit Transdermal 5 g/kg |
| 4 | <i>o</i> -Xylene (oX) |  | Colorless transparent; Liquid Aromatic odor | (1) BP: 144.4 °C (2) MP: -25.2°C (3) 0.178g/1L Water; Soluble in ethanol, ether, chloroform and other organic solvents (4) LogP: 3.14 | 2.63 | 14.1 | Carcinogen: Group 3 Human inhalation 6125 ppm/12h Rat oral 5 mg/kg |
| 5 | <i>m</i> -Xylene (mX) |  | Colorless transparent liquid; Smell similar to toluene | (1) BP: 139.1°C (2) MP: -47.9 °C | 2.63 | 14.1 | Carcinogen: Group 2B LD50 : Rat transoral 5000 mg/kg |

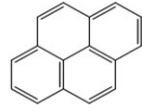
| | | | | | | | |
|----|--------------------------|---|---|---|------|------|--|
| 6 | <i>p</i> -Xylene (pX) |  | Colorless liquid; Colorless lamellar or prismatic crystal | (3) 0.162 g/1L Water; Soluble in ethanol, ether, chloroform and other organic solvents (4) LogP: 3.14 (1) BP: 139.61 °C (2) MP: 13.26 °C (3) 0.198 g/1L Water; Soluble in ethanol, ether, chloroform and other organic solvents (4) LogP: 3.14 | 2.63 | 14.1 | Rabbit transdermal 14100 mg/kg Rat intraperitoneal 1739 mg/kg Carcinogen: Group 3 |
| 7 | Benzenamine |  | Colorless to light yellow transparent liquid | (1) BP: 184 °C (2) MP: -6.3 °C (3) 3.6 g/0.1L Water (20 °C) Soluble in ethanol, ether and other organic solvents (4) LogP: 1.23 | 5.92 | 32.5 | Carcinogen: Group 3 Rat intraperitoneal 420 mg/kg Mouse intraperitoneal 492 mg/kg |
| 8 | Styrene |  | Colorless and transparent oily liquid Aromatic odor | (1) BP: 145 °C (2) MP: -31 °C (3) Soluble in alcohol, ether and other organic solvents (4) LogP: 2.03 | 36.5 | 235 | Carcinogen: Group 2B LD50: Rat transoral 5000 mg/kg LC50: Rat inhalation 24000 mg/m3, 4h |
| 9 | Nitrobenzene |  | Colorless or yellowish oily liquid Bitter almond flavor | (1) BP: 210.9 °C (2) MP: 5.7 °C (3) 1.9 g/1L Water (20 °C); Density greater than water Soluble in ethanol, ether, benzene and oil (4) LogP: 1.83 | 0.99 | 4.25 | Carcinogen: Group 2B LD50: Rat transoral 489 mg/kg Rat transdermal 2100 mg/kg Human (female) transoral 200mg/kg |
| 10 | 2,4-Dinitrotoluene |  | Yellow needle crystal Monoclinic prism Industrial product is an oily liquid | (1) BP: 300 °C (2) MP: 65.5-70.5 °C (3) Soluble in benzene; Slightly soluble CS ₂ ; Slightly soluble in ether, cold ethanol; Very slightly soluble in | 1.54 | 4.68 | Carcinogen: Group 2B LD50: Rat oral 268 mg/kg Mouse oral 790 mg/kg |

| | | | | | | | |
|--|----------------------------|---|---|---|-------|------|--|
| 11 | Chlorobenzene |  | Colorless liquid Bitter almond flavor | water (4) LogP: 2.2 (1) BP: 132.2 °C (2) MP: -45 °C (3) 0.049 g/100g Water (30 °C); Soluble in ethanol, ether, chloroform, CS ₂ , benzene and other organic solvents (4) LogP: 2.52 | 1.31 | 7.06 | Carcinogen: Group 3 LD50: Rat transoral 2290 mg/kg Mouse transoral 1445mg/kg |
| 12 | 1,2-Dichlorobenzene |  | Colorless and volatile liquid Aromatic odor | (1) BP: 180.4 °C (2) MP: -17.5 °C (3) Soluble in most organic solvents such as alcohol and ether; Insoluble in water (4) LogP: 2.52 | 11.4 | 73.5 | Carcinogen: Group 2B LD50: Rat subcutaneous 5mg/kg Rabbit intravenous 400 mg/kg |
| 13 | 1,4-Dichlorobenzene |  | White crystal Irritating smell | (1) BP: 174 °C (2) MP: 53.1 °C (3) Soluble in ethanol, ether, benzene and other organic solvents Insoluble in water (4) LogP: 3.15 | 0.079 | 0.39 | Carcinogen: Group 2B LD50: Rat transoral 500 mg/kg |
| B) Polycyclic aromatic hydrocarbons (USEPA) | | | | | | | |
| 14 | *Naphthalene (Nap) |  | A white crystalline volatile solid with a strong coal-tar | (1) BP:217.9 °C (2) MP:80.5 °C (3)1 g/13ml ethanol or methanol; Very soluble in ether hydronaphthalenes and in fixed and volatile oils (4) LogP: 3.3 | 0.48 | 2.13 | Carcinogen: Group 2B LD50: Guinea pig oral 1200 mg/kg Mouse intraperitoneal 150 mg/kg and oral 316 mg/kg Rat oral 490 mg/kg Rabbit oral 3000 mg/kg |
| 15 | *1,2-Benzanthrene (BaA) |  | Colorless solid and solutions have a slight blue fluorescence | (1) BP:437.6 °C (2) MP:162 °C (3) In water,0.0094 mg/L at 25 °C | 0.63 | 1.86 | Carcinogen: Group 2B LD50: Rat intraperitoneal >200 mg/kg |

| | | | | | | | |
|----|--------------------------------------|---|--|--|-------|------|---|
| 16 | *Benzo[a]pyrene (BaP) |  | Colorless to yellowish acicular crystal | (4) LogP: 5.76 (1) BP:496 °C (2) MP:178.3 °C (3) In water,0.00162 mg/L at 25 °C Slightly soluble in ethanol and methanol | 0.064 | 0.19 | Carcinogen: Group 1 LD50: Rat subcutaneous 50 mg/kg |
| 17 | *Benzo[b]fluoranthene (BbF) |  | Needles or yellow fluffy powder | (4) LogP: 5.34 (1) BP:481 °C (2) MP:168 °C (3) 0.0015 mg/1L in Water | 0.64 | 1.87 | Carcinogen: Group 2B |
| 18 | *Benzo[k]fluoranthene (BkF) |  | Pale yellow needles or yellow crystalline solid Neat | (4) LogP: 5.34 (1) BP:480 °C (2) MP:216 °C (3) 95% ethanol: <1 mg/mL at 20°C;1.09 µg/L at 25 °C | 6.2 | 18 | Carcinogen: Group 2B |
| 19 | Chrysene (Chr) |  | White or silvery gray yellow green scales green scales or orthorhombic Forming colorless rhombic lamellae in benzene Purple fluorescence under UV | (4) LogP: 6.11 (1) BP:448 °C (2) MP:253 °C (3) 1 g/1.3L anhydrous ethanol;1 g/0.48L methanol (25 °C) Dissolve about 5% in toluene at 100 °C; insoluble in water. | 61.5 | 178 | Carcinogen: Group 2B LD50: Mouse intraperitoneal >320 mg/kg |
| 20 | Dibenzo[a,h]anthracene (DBahA) |  | White crystals or pale yellow solid | (4) LogP: 6.03 (1) BP:524 °C (2) MP:259 °C (3) In water,0.00249 mg/L at 25 °C | 0.064 | 0.19 | Carcinogen: Group 2B |
| 21 | *Indeno[1,2,3-cd]pyrene (InP/IcP) |  | Yellow flaky or needle-like crystals Light green fluorescence | (4) LogP: 5.66 (1) BP:536 °C (2) MP:164 °C (3) 0.6 mg/2ml lolive oil;0.0062 mg/L Water (20 °C) | 0.64 | 1.87 | Carcinogen: Group 2B Carcinogen: Group 3 |

| | | | | | |
|----|--------------------------------|---|---|--|--|
| 22 | *Benzo[g,h,i]perylene (BgP) |  | Colorless to white crystalline solid | (1) BP: 550 °C (2) MP:278.3 °C (3) In water, 0.00026 mg/L at 25 °C (4) LogP: 6.50 | |
| 23 | Acenaphthene (Ace) |  | White needle- like crystals | (1) BP:279 °C (2) MP:95 °C (3) In water, 3.90 mg/L at 25 °C (4) LogP: 3.92 | Carcinogen: Not listed LD50: Rat intraperitoneal 600 mg/kg |
| 24 | Acenaphthylene (Acy) |  | Yellow prismatic or plate-like crystals | (1) BP:78 °C (2) MP:280 °C (3) In water, 3.93 mg/L at 25 °C (4) LogP: 3.93 | Carcinogen: Group 3 LD50: Mouse oral 1760 mg/kg Rat intraperitoneal 1700 mg/kg |
| 25 | Fluorene (Fl) |  | White flaky crystals | (1) BP:294 °C (2) MP:114.77 °C (3) In water, 1.69 mg/L at 25 °C (4) LogP:4.18 | Carcinogen: Group 3 LD50: Mouse intraperitoneal >2000 mg/kg |
| 26 | Phenanthrene (Phe) |  | Colorless monoclinic crystals with a faint aromatic odo | (1) BP:340 °C (2) MP:97~101 °C (3) In water, 1.10 mg/L at 25 °C (4) LogP:4.46 | Carcinogen: Group 3 LD50: Mouse intraperitoneal 700 mg/kg and oral 700 mg/kg |
| 27 | Anthracene (Ant) |  | Pale yellow needle- like crystals with blue fluorescence | (1) BP:340 °C (2) MP:215 °C (3) In water, 0.0434 mg/L at 24 °C (4) LogP:4.45 | Carcinogen: Group 3 LD50: Mouse vein 430 mg/kg |
| 28 | *Fluoranthene (Flu) |  | Yellow-green needle-like or flaky crystals | (1) BP:384 °C (2) MP:110 °C (3) Virtually insoluble (0.20-0.26 mg/L) in water (4) LogP:5.16 | Carcinogen: Group 3 LD50: Mouse intraperitoneal 100 mg/kg; Rat oral 2000 mg/kg |

29 Pyrene
(Pyr)



Pale yellow monoclinic
crystals

- (1) BP:393.5 °C
- (2) MP:156 °C
- (3) In water, 0.135mg/L at 24 °C
- (4) LogP:4.88

Carcinogen: Group 3
LD50: Mouse intraperitoneal
514 mg/kg and oral 800 mg/kg
Rat oral 2700 mg/kg
