POLYCYCLIC AROMATIC HYDROCARBONS (PAH)

Identity

Name (parent)	Polycyclic aromatic hydrocarbons (PAHs)
UN number	n/a
CAS number	130498-29-2
Intervention value (mg/m^3)	n/a
Structure	Group of over 100 chemicals: organic substances made up of carbon and hydrogen atoms grouped into at least two condensed aromatic ring structures

Occurrence

Chemical state (at 20°C)	Solid
Physical appearances	Colorless, white, or pale yellow-green solids
Industrial products	Creosote; coal coking; production of aluminum, steel and iron; used as intermediate in the synthesis of several industrial products (e.g. dyes and pesticides); present in coal tar; product of incomplete combustion

Physicochemical properties

Molecular weight	Several compounds: range 128.2 (naphtalene) to 506.6 (hexabenzo[a,c-d,f,j,l-m,o]perylene; $C_{42}H_{22}$)
Vapor pressure (mbar at 25°C)	Low vapor pressure: 0.10 (naphtalene) - $2 * 10^{-12}$ (coronene) mbar
Octanol/water partition coefficient (log Po/w)	Relatively high (highly lipophilic): e.g. 3.3 (naphtalene) - 5.97 (benzo[a]pyrene) - 6.84 (dibenz[a,h]anthracene) - 7.30 (coronene)
Water solubility (in mg/L at 25 °C)	Low to insoluble: e.g 0.135 mg/L for pyrene, $1.6 *10^{-3}$ mg/L for benzo[a]pyrene

Toxicokinetics (parent)

Uptake by inhalation	Deposition of ultrafine particles derived from combustion sources. Influenced by carrier particles and solubility of the PAH, extent of absorption not known [1].
Uptake by skin absorption	Extent of absorption variable among the different compounds and is affected by the vehicle of administration [1]. In coke oven workers of the skin contamination with pyrene 75% (28-95%) and of skin contamination with benzo[a]pyrene 51% (8-92%) was absorbed [2].
Uptake via gastrointestinal tract	Dependent on lipophilicity: oral absorption increases with more lipophilic compounds or in the presence of oils in the GI tract [1].
Distribution	Distributed rapidly to highly perfused organs, accumulates in fatty tissues.
Metabolism	Phase 1 (among others CYP 450) and phase 2 metabolism.
Excretion via lungs	Not common due to low vapor pressure.
Excretion via urine	Low molecular weight PAHs (3 or fewer aromatic rings) [3].
Excretion via feces	Main excretion route for PAHs; PAHs with higher molecular weight (more than 3 aromatic rings) [3].

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Toxicodynamics

Mechansisms of toxicity	Formation of reactive metabolites (e.g epoxides) which covalently bind to DNA explaining genotoxity. PAHs are also phototoxic.
Classifications for carcinogenicity	IARC classifications range from human carcinogen (benzo[a]pyrene, group 1); to probably carcinogenic to humans (dibenz[a,h]anthracene, group 2A); to possibly carcinogenic to humans (benz[a]anthracene, group 2B) to not classifiable (pyrene, group 3) [4]
Classifications for reprotoxicity	Benzo[a]pyrene is reprotoxic in animals [1]
Classifications for sensitizing properties	Benzo[a]pyrene is a skin sensitizer [5]

Biological monitoring

Biomarkers	**1-hydroxypyrene in urine (1-OHP)**
Molecular weight	218.3
Involved enzymatic metabolism	Cytochrome P450 (most important: CYP1A1, CYP1B1, CYP1A2); glucuronisyltransferase (glucuronidation of 1-OHP)
Biological material	Urine
Type of sample	Spot urine
Sampling strategy	Collection of several spot samples over 1-2 days / collection of 24 hour urine
Half life of excretion	Triphasic urinary elimination: $T_{1/2}$ is 5 hours, 22 hours and 17 days [6]
	First-order kinetics
Materials	Polystyrene universal container (30 mL)
Transportation	At 4°C, within 24 hours
Storage	-20°C (> 6 month)
Stability	At 4°C for 24 h; at -20°C for > 6 month
Measurement principle	HPLC and fluorescence; GC-MS
Limit of quantification	2 µg/L (limit of determination)
Aliquot for 1 analysis	5 mL (collection) / 2 mL (for analysis)
Recommended adjustments	Use creatinine for correction of urine density
Preferred units for expression of results	µmol 1-OHP / mol creatinine (spot urine) or µmol 1-OHP / 24 h
Conversion factor	1 µmol 1-OHP/ mol creatinine = 1.929 µg/g creatinine 1 µmol 1-OHP / 24 hours = 218.3 µg / 24 h
Biological exposure value US	0.49 µmol 1-OHP/ mol creatinine (at end-of-shift and end-of-workweek). Workers with a value above this level should be classified as occupationally exposed [7]. If pyrene and benzo[a]pyrene was measured from air, surface or skin samples the following adjustment may be made: 1 µg 1-OHP/ L = (pyrene/benzo[a]pyrene)/2.5. The proposed value has a 'Nq notation' because of lack of quantitative relationship with exposure [7].
Biological Limit Values Germany (workers)	Not available
BIOMONECS background in non-smoking m/f adults (based on P0.95)	0.09 µmol 1-OHP/ mol creatinine [8]
Reference value	< 2 µg/ g creatinine [9]
Possible confounders	Use of coal tar products (tar shampoo, wood preservatives, creosote), smoking, diet (consumption grilled products)

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