Annex XV dossier

PROPOSAL FOR IDENTIFICATION OF A SUBSTANCE AS A CMR CAT 1 OR 2, PBT, vPvB OR A SUBSTANCE OF AN EQUIVALENT LEVEL OF CONCERN

Substance Name: Anthracene oil

EC Number: 292-602-7

CAS Number: 90640-80-5

Submitted by: Germany

Version: August 2009

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PROPOSAL FOR IDENTIFICATION OF A SUBSTANCE AS A CMR CAT 1 OR 2, PBT, vPvB OR A SUBSTANCE OF AN EQUIVALENT LEVEL OF CONCERN

Substance Name: Anthracene oil

EC Number: 292-602-7

CAS Number: 90640-80-5

- It is proposed to identify the substance as a PBT according to Article 57 (d).
- It is proposed to identify the substance as a vPvB according to Article 57 (e).

Summary of how the substance meets the CMR (Cat 1 or 2), PBT or vPvB criteria, or is considered to be a substance of an equivalent level of concern

Anthracene oil is a UVCB substance consisting of different constituents, among them various PAH. One relevant constituent is anthracene which is present in anthracene oil in the range of 3-25 %. Anthracene has been placed on the Candidate List due to the identification as a PBT-substance. Moreover, anthracene oil consists of further PAH in concentrations above 0.1% (w/w) such as phenanthrene, fluoranthene and pyrene. These three PAH fulfil the PBT and vPvB criteria, too.

Hence, anthracene oil fulfils the PBT, and the vPvB, criteria according to article 57 d) and e) of the REACH regulation.

Registration number(s) of the substance or of substances containing the substance:

JUSTIFICATION

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Chemical Name:Anthracene oilEC Number:292-602-7CAS Number:90640-80-5IUPAC Name:

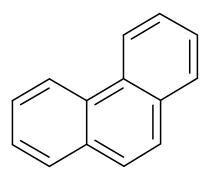
1.2 Composition of the substance

The anthracene oil derivates are complex and have variable compositions. Anthracene oil (CAS-No: 90640-80-5) is an UVCB substance consisting of three- to five-membered condensed aromatic hydrocarbons. It is an oily liquid with a colour ranging from yellow over dark green to brown and it is produced during the distillation of coal tars. Coal tars are the condensation products obtained by cooling of the gas evolved in the carbonization of coal. The relative proportions of the constituents of anthracene oil are complex and variable and dependent on whether low temperature or high temperature processes were involved in the production of the tar. Over 400 constituents have been identified in coal tars, and probably as many as 10,000 are actually present (International Agency for Research on Cancer (IARC), 1985). The number of constituents present in most anthracene oils is estimated in the hundreds.

According to the EC inventory anthracene oil is a complex combination of polycyclic aromatic hydrocarbons obtained from coal tar having an approximate distillation range of 300°C to 400°C (572°F to 752°F). It is composed primarily of phenanthrene, anthracene and carbazole. The data provided by industry in the IUCLID files is shown in the list below.

Chemical Name:
EC Number:
CAS Number:
IUPAC Name:
Molecular Formula:
Structural Formula:

Phenanthrene 201-581-5 85-01-8 Phenanthrene C14H10



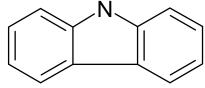
Molecular Weight:178.23Typical concentration (% w/w):10 - 35

Chemical Name:	Fluoranthene
EC Number:	205-912-4
CAS Number:	206-44-0
IUPAC Name:	Fluoranthene
Molecular Formula:	C16H10
Structural Formula:	
Molecular Weight:	202.26
Typical concentration (% w/w):	
Concentration range (% w/w):	2 - 15
Chemical Name:	Pyrene
EC Number:	204-927-3
CAS Number:	129-00-0
IUPAC Name:	Pyrene
Molecular Formula:	C16H10
Structural Formula:	
Molecular Weight:	202.26
Typical concentration (% w/w):	
	1 10

Concentration range (% w/w): 1 - 10

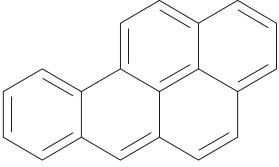
Chemical Name:	Fluorene
EC Number:	201-695-5
CAS Number:	86-73-7
IUPAC Name:	9H-fluorene
Molecular Formula:	C13H10
Structural Formula:	
Molecular Weight:	166.22
Typical concentration (% w/w):	
Concentration range (% w/w):	1 - 16
Chemical Name:	Anthracene
	1 mmueene
EC Number:	204-371-1
EC Number: CAS Number:	
	204-371-1
CAS Number:	204-371-1 120-12-7
CAS Number: IUPAC Name:	204-371-1 120-12-7 Anthracene
CAS Number: IUPAC Name: Molecular Formula:	204-371-1 120-12-7 Anthracene
CAS Number: IUPAC Name: Molecular Formula: Structural Formula:	204-371-1 120-12-7 Anthracene C14H10
CAS Number: IUPAC Name: Molecular Formula: Structural Formula: Molecular Weight:	204-371-1 120-12-7 Anthracene C14H10

Chemical Name:	Carbazole
EC Number:	201-696-0
CAS Number:	86-74-8
IUPAC Name:	9H-carbazole
Molecular Formula:	C12H9N
Structural Formula:	н
	\wedge \dot{N} \wedge



Molecular Weight: 167.21 Typical concentration (% w/w): Concentration range 1 – 10 (% w/w):

Chemical Name:	Benzo(a)pyrene (BaP)
EC Number:	200-028-5
CAS Number:	50-32-8
IUPAC Name:	Benzo[def]chrysene; benzo[pqr]tetraphene
Molecular Formula:	C20H12
Structural Formula:	\sim \sim



Molecular Weight: 252.32 Typical concentration (% w/w):

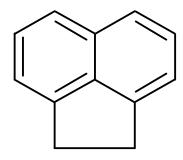
< 0.05

Concentration range (% w/w):

Chemical Name: EC Number: CAS Number: IUPAC Name: Molecular Formula:

Structural Formula:

Acenaphthene
201-469-6
83-32-9
1,2 dihydroacenaphthylene
C12H10



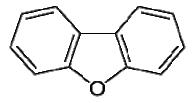
Molecular Weight:	154.21
Typical concentration (% w/w):	
Concentration range (% w/w):	0.2 - 16

Chemical Name: EC Number: CAS Number: IUPAC Name: Molecular Formula:

Structural Formula:

205-071-3 132-64-9 Dibenzo[b,d]furan C12H8O

Dibenzofuran



Molecular Weight: 168,19

Typical concentration (% w/w):

Concentration range (% w/w): 0.1-8

1.3 Physico-chemical properties

REACH ref Annex, §	Property	IUCLID section	Value	Comment/reference
VII, 7.1	Physical state at 20°C and 101.3 kPa	4.1	Solid, liquid	IUCLID datafile
VII, 7.2	Melting/freezing point	4.2	< 80 °C	IUCLID datafile
VII, 7.3	Boiling point	4.3	> 270 °C	IUCLID datafile
VII, 7.5	Vapour pressure	4.6	< 1 hPa at 20°C	
VII, 7.7	Water solubility	4.8	0.041 – 1,98 mg/l	IUCLID datafile; Depending on the concentration of the different substances
VII, 7.8	Partition coefficient n- octanol/water (log value)	4.7 partition coefficient	3,45 - 4,8	IUCLID datafile; Depending on the concentration of the different substances

Table 1: Summary of physico-chemical properties

2 MANUFACTURE AND USES

Not relevant for this type of dossier.

3 CLASSIFICATION AND LABELLING

3.1 Classification in Annex VI of Regulation (EC) No 1272/2008

Anthracene oil has index number 648-079-00-6 in Annex VI, part 3, Tables 3.1 and 3.2 of Regulation (EC) No 1272/2008.

Its classification according to part 3 of Annex VI, Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008 and of its constituents addressed in this dossier is provided in Table 2.

Table 2: Classification and labelling of anthracene oil and its constituents according to Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008.

Name	CAS-No	Index-No	Classification	Labelling
Anthracene Oil [#]	90640-80-5	648-079-00-6	Carc. Cat. 2; R45*	T; R45; S 53 – 45
Benzo(a)pyrene	50-32-8	601-032-00-3	Carc. Cat 2; R45 ^{\$} Muta. Cat. 2; R46 Repr.Cat 2; R60-61; R43 N; R 50-53	T; N R: 45 ^{\$} -46-60-61-43- 50/53 S: 53-45-60-61

[#]The classification and label shown for this substance applies to the dangerous property indicated by the risk phrases in combination with the category of danger shown. Manufacturers, importers and downstream users of this substance shall be obliged to carry out an investigation to make themselves aware of the relevant and accessible data which exists for all other properties to classify and label the substance. The final label shall follow the requirements of section 7 of Annex VI to Directive 67/548/EEC;* The classification as a carcinogen need not apply if it can be shown that the substance contains less than 0,005 % w/w benzo[a]-pyrene (EINECS No 200-028-5). [§] Concentration Limit ≥ 0.01 %

The harmonised classification and labelling of anthracene oil and its constituents as hazardous substances according to Regulation (EC) No 1272/2008 (Annex VI, part 3, Table 3.1) is provided in Table 3.

Name	CAS-No	Index-No	Classification	Labelling
Anthracene Oil [#]	90640-80-5	648-079-00-6	Carc. Cat. 1B [*] H350	GHS08 Dgr H350
Benzo(a)pyrene	50-32-8	601-032-00-3	Carc. 1B ^{\$} Muta. 1B Repr. 1B Skin Sens. 1 Aquatic Acute 1 Aquatic Chronic1 H350 ^{\$} ; H340; H360- FD; H317 : H400; H410	GHS08; GHS07; GHS09; Dgr H350 ^{\$} ; H340; H360FD; H317; H410

Table 3: Classification and labelling of anthracene oil and its constituents according to Annex VI, part 3, Table 3.1 of Regulation (EC) No 1272/2008.

[#] The classification and labelling shown for this substance applies to the hazardous property(ies) indicated by the hazard statement(s) in combination with the hazard class(es) and category(ies) shown. The requirements of Article 4 (Regulation (EC) No. 1272/2008) for manufacturers, importers or downstream users of this substance apply to all other hazard classes and categories.; *The classification as a carcinogen need not apply if it can be shown that the substance contains less than 0,005 % w/w benzo[a]-pyrene (EINECS No 200-028-5).; *Specific Concentration Limit ≥ 0.01 %

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation

4.1.1 Stability

4.1.1.1 Phototransformation

Photolysis in the troposphere results in the formation of reactive hydroxyl (OH) and nitrate (NO₃) radicals and ozone (O₃), which react as oxidizing agents with organic compounds, like PAHs. These radical and ozone reactions comprise mainly the degradation of gas-phase PAH (Calvert et al., 2002). The atmospheric behaviour of the main constituents of anthracene oil¹ is shown below in Table 4.

Table 4: Phototransformation of the main constituents present in anthracene oil. Data aretaken from the Annex XV transitional report for coal tar pitch, high temperature (TheNetherlands - Bureau REACH, 2009)

	Representative lifetime in air with respect to reaction with								
PAH (number of rings)		ОН	NO ₃	O ₃					
	Summer	Winter							
Phenanthrene (2)	9.0 h	1.9 d	-	-					
Fluoranthene (4)	5.6 h	1.2 d	340 d	-					
Fluorene (3)	1.8 d	9 d	-	-					
Pyrene (4)	5.6 h	1.2 d	120 d	-					
Acenaphthene (3)	3.5 h	18 h	4.8 h	> 30 d					
Carbazole (2) ^{a)}	9.6 h	-	-	-					
Dibenzofuran (2) ^{a)}	2.7 d	-	-	-					
Benzo(a)pyrene (5) ^{a)}	7.7 h	-	-	-					

a) Especially calculated for this dossier with AOPwin v1.91

For all these substances the transformation rate in the particle phase is expected to be slower. Particle phase transformation is, however, not assumed to be of relevance for the overall atmospheric lifetime, because e.g. only up to 3% of atmospheric anthracene has been observed to appear in particle phase (European Chemicals Agency, 2008d).

Environmentally relevant exposure occurs in the whole water column and, in the case of the constituents of anthracene oil, especially in sediment and soil. Photodegradation can be expected to be a relevant removal pathway in the environment only in very shallow clear waters and in the first

¹ Please note that data relevant for the constituent anthracene are not shown in this dossier, since anthracene has already been identified as a PBT substance (European Chemicals Agency, 2008d).

few centimetres layer of the water column. Therefore aquatic photodegradation is not considered to have relevant impact on the overall persistency of anthracene oil in the environment.

4.1.1.2 Hydrolysis

Hydrolysis as a way of abiotic degradation can be considered as not relevant for the main constituents of the UVCB substance anthracene oil because of their chemical structures. E.g. the constituent anthracene is stable against hydrolysis and photochemical transformation in water and sediments. This has been observed in laboratory and in "in situ" experiments. Half-lives for primary photodegradation in water have been reported in the range of 20 minutes to 125 hours depending on the experimental conditions used. The highest value corresponds to photolysis in winter conditions. Anthraquinone has been identified as the main abiotic degradation product of anthracene (European Chemicals Agency, 2008d). Because of the similar chemical structure (consisting of aromatic rings) similar assumptions for hydrolytic behaviour of the other anthracene oil constituents can be made (MITI-List, 2002).

4.1.2 Biodegradation

4.1.2.1 Biodegradation estimation

4.1.2.2 Screening tests

The PAH listed in Table 5 were allocated to persistence classes on the basis of model calculations (Mackay et al., 1992). The half-lives were applied in the Annex XV transitional report of coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Table 5: Ranking of PAH in different half-life classes according to (The Netherlands - Bureau REACH, 2009)

Substance		Water	Soil		Sediment	
	class	Half-life [d]	class	class Half-life [d]		Half-life [d]
Acenaphthene	3	5 – 13	5	42 - 125	6	125 - 420
Fluorene	4	13 - 42	6	125 - 420	7	420 - 1250
Phenanthrene	4	13 - 42	6	125 - 420	7	420 - 1250
Fluoranthene	4	13 - 42	7	420 - 1250	8	>1250
Pyrene	5	42 - 125	7	420 - 1250	8	>1250

In a 28 day ready biodegradability test (MITI I, OECD 301C) using 100 mg I^{-1} PAH, respectively, and 30 mg I^{-1} sludge readily biodegradation was detected for phenanthrene. For fluorene, carbazole, acenaphthene and dibenzofuran no biodegradation was measured (see Table 6). According to the MITI test, which is suitable for substances with low water solubility, these PAH are not readily biodegradable

Substance	BOD	Judgement
Phenanthrene	54,0	Ready biodegradable
Fluorene	0 %	Not-biodegradable
Carbazole	0 %	Not-biodegradable
Acenaphthene	0%	Not-biodegradable
Dibenzofuran	1%	Not-biodegradable

Table 6: Biodegradation of several PAH according to the test method MITI I (OECD TG301C).

Coover and Sims tested the persistence of PAHs in an unacclimated agricultural sandy loam soil in dependence of the temperature (Coover and Sims, 1987). Due to the method used for extraction and analysis, it remains unclear to which extent evaporation, adsorption and biodegradation may have contributed to the elimination process. The soil was spiked with a standard solution of 16 PAHs and incubated for 240 days. At 10°C 36% of phenanthrene, 94% of fluoranthene and 93% of pyrene were remaining. With increasing temperature the degradation increased. 19% (2%) of phenanthrene, 71% (15%) of fluoranthene and 89% (43%) of pyrene were remaining at 20°C (30°C).

4.1.2.3 Simulation tests

Biodegradation in soil

Biodegradation rates of several PAH in soil depend on several factors like soil type, pH, moisture content, oxygen and nutrient contents and soil microbial population. In addition, vegetation has been observed to enhance microbial biodegradation in the rhizosphere. Some of these factors may also explain why the half-lives observed under laboratory conditions are much shorter than those obtained from long-term field-based experiments (The Netherlands - Bureau REACH, 2009). The results of Wild et al. (1991) and Wild and Jones (1993) demonstrate the difference of tests conducted for several PAHs in field conditions compared to laboratory tests. Wild et al. (1991) observed elimination half-lives of 5.7 years for phenanthrene, 7.8 years for fluoranthene, and 8.5 years for pyrene. In this field experiment soils were enriched with PAH-contaminated sludge (Wild et al., 1991).

In another study Wild and Jones (1993) derived different half-lives in a microcosm study with four soil types (Wild and Jones, 1993). The elimination half-lives for the PAH tested are as follows: phenanthrene 83 - 193 days; fluoranthene 110 - 184 days; and pyrene 127 - 320 days. It has to be noted that the latter results are derived from a greenhouse study and should therefore not be used for the P-assessment. Various studies on PAH-contaminated soils have shown that the number of PAH-degrading microorganisms and the degrading capacity are much higher in PAH-contaminated soils than in pristine soils indicating that adaptation has occurred (The Netherlands - Bureau REACH, 2009; European Commission, 2008).

Grosser et al. studied the mineralization of ¹⁴C-labeled pyrene and carbazole in three different soils (Grosser et al., 1991). The mineralization was measured by application of serum bottle radiorespirometry. The incubation was set up for 184 days, but after 60 days the curves had become asymptotic. The mineralization of pyrene was measured between 10 and 48% and for carbazole between undetectable and 46% within the test duration.

The fate of several PAHs in two different soils were tested by Park et al. (Park et al., 1990). The half-life of phenanthrene was calculated as being in the range of 27 and 53 days (second soil: 13 - 18 days), whereas the half life of fluoranthene ranged between 173 and 630 days (second soil: 277 - 578 days) and that of pyrene between 131 and 408 days (second soil: 193 - 408 days).

Substance	Result	Reference
Phenanthrene	$DisDT_{50} = 5.7$ years(field study)	(Wild et al., 1991)
	DisDT ₅₀ =83 – 193 d (microcosm study)	(Wild and Jones, 1993)
	Elimination half- life in two different soils:	(Park et al., 1990)
	$DisDT_{50} = 27 - 53 d$ $DisDT_{50} = 13 - 18 d$	
Fluoranthene	$DisDT_{50} = 7.8$ years (field study)	(Wild et al., 1991)
	$DisDT_{50} = 110 - 184 d \text{ (microcosm study)}$	(Wild and Jones, 1993)
	Elimination half- life in two different soils:	(Park et al., 1990)
	$DisDT_{50} = 173 - 630 d$ $DisDT_{50} = 277 - 578 d$	
Pyrene	Degradation half-life: DegDT ₅₀ > 184 d (10 – 48% mineralization in 184 d)	(Grosser et al., 1991)
	DisDT ₅₀ = 8.5 years (field study)	(Wild et al., 1991)
	DisDT ₅₀ =167 - 320 d	(Wild and Jones, 1993)
	Elimination half- life in two different soils:	(Park et al., 1990)
	$DisDT_{50} = 131 - 408 d$	
Carbazole	DisDT ₅₀ = $193 - 408$ d Degradation half-life: DegDT ₅₀ > 184 d (undetectable - 46%	(Grosser et al., 1991)
	mineralization in 184 d)	

Table 7: Half-lives in soil of relevant constituents of anthracene oil

4.1.3 Summary and discussion of persistence

Anthracene, which is one relevant constituent of anthracene oil, has been placed on the Candidate List due to the identification as a PBT-substance (European Chemicals Agency, 2008d).

Moreover, anthracene oil consists of further hardly degradable PAH constituents. The model calculations by Mackay et al. (1992) indicate that acenaphtene, fluorene, phenanthrene, fluoranthene, and pyrene show half-times in sediment > 180 days.

Screening studies (OECD TG 301C) show, that acenaphtene, fluorene, carbazole, and dibenzofuran – constituents present in anthracene oil - are not readily biodegradable (MITI-List, 2002).

Further studies show relatively long dissipation times for fluoranthene (DisDT₅₀ > 173 d), pyrene (DisDT₅₀ > 131 d), and carbazole (DegDT₅₀ > 184 d) (Park et al., 1990; Grosser et al., 1991).

Additionally in a field study half-lives of 5.7 years for phenanthrene, 7.8 years for fluoranthene, and 8.5 years for pyrene, have been measured in soil (Wild et al., 1991).

Hence, several constituents of anthracene oil fulfil the P and/or the vP criteria according to article 57 d) and e) of the REACH regulation.

4.2 Environmental distribution

4.2.1 Adsorption/desorption

The organic carbon partitioning coefficient log K_{OC} was calculated for the main constituents using the equation $log K_{OC} = 0.81 * log K_{OW} + 0.10$ (European Chemicals Agency, 2008b). The results are shown below in Table 8.

Substance	CAS-No.	logK _{OW} ^{a)}	logK _{OC}	$K_{OC} (l/kg)^{b}$
Phenanthrene	85-01-8	4.57	3.80	6,309
Fluoranthene	206-44-0	5.20	4.31	20,417
Fluorene	86-73-7	4.22	3.52	3,311
Pyrene	129-00-0	4.98	4.13	13,489
Acenaphthene	83-32-9	4.00	3.34	2,187
Carbazole	86-74-8	3.84	3.21	1,621
Dibenzofuran	132-64-9	5.16	4.28	19,054

Table 8: LogK_{OW} and logK_{OC} data of the relevant constituents of anthracene oil

a) Values taken from Annex XV transitional report – CTPHT (The Netherlands - Bureau REACH, 2009); b) calculation of K_{OC} according to Guidance document R.7a

It can be concluded that anthracene oil has a high potential to adsorb to organic matter and that it is not or only little mobile in soil and sediment.

4.2.2 Volatilisation

For the substance anthracene oil no measured data are available at the moment. According to the constituents' Henry' Law constants anthracene oil is appreciated to be moderately volatile. The calculated values are shown in Table 9 using the equation for Henry's law constant documented in Guidance Document R.16 (European Chemicals Agency, 2008b).

4.2.3 Distribution modelling

For the main constituents of anthracene oil the behaviour in the wastewater treatment plant was calculated under the assumption that no biodegradation occurs (k=0/h). The results are shown in Table 9.

Table 9: Henry constants and volatilisation of main constituents in municipal waste water	
treatment plants.	

Substance	Henry- constant ^a	Distribution of PAH in STP ^b					
	(Pa*m³/mol)	% to air	% to water	% to sludge	% degraded		
Phenanthrene	4.76	4.4	53.5	42.1	0.0		
Fluoranthene	0.14	0.6	31.7	67.7	0.0		

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Fluorene	7.57	8.5	63.6	27.9	0.0
Pyrene	1.62	1.1	39.3	59.6	0.0
Acenaphthene	13.01	14.5	65.2	20.3	0.0
Carbazole	0.01	0.0	83.3	16.7	0.0
Dibenzofuran	24.21	8.9	27.4	63.7	0.0

^acalculation of Henry's law coefficient according to Guidance Document R.16 (European Chemicals Agency, 2008c); ^b values for distribution in STP calculated with SimpleTreat 3.0 (debugged version, 7 Feb 97)

Due to the partitioning to solids, low to medium concentrations of these PAHs in aqueous solutions are expected. The share of volatilised anthracene oil constituents depends on the composition of the oil. Nevertheless volatilisation is not considered as a relevant route of distribution for anthracene oil.

4.3 Bioaccumulation

4.3.1 Aquatic bioaccumulation

4.3.1.1 Bioaccumulation estimation

Based on the substance's log K_{OW} range from 3.84 to 6.06, constituents of anthracene oil are expected to bioaccumulate.

4.3.1.2 Measured bioaccumulation data

Bioaccumulation of various PAH has been measured in various species. Several studies have been discussed in detail in the risk assessment report of anthracene (de Maagd, 1996; de Voogt et al., 1991; Djomo et al., 1996) and in the Annex XV transitional report for coal tar pitch, high temperature (McLeese et al., 1987; Petersen and Kristensen, 1998; Bruner et al., 1994). The most relevant studies and results are summarized in the following table.

Substance	Species	BCF	R ^{a)}	Test system ^{b)}	Type ^{c)}	References
Fluorene	Fish					
	Poecilia reticulata	2230	3	S	k1/k2 (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	1050	2	R	equilibrium (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	3500	2	S	equilibrium (parent)	(de Voogt et al., 1991)
Phenanthrene	Fish					
	Brachydanio rerio (eggs)	9120 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio (eggs)	12303 ^d)	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio (larvae)	7943 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio (larvae)	6309 ^d	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Gadus morhua (larvae)	10715 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Gadus morhua (larvae)	14454 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Clupea harengus (larvae)	20893 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Clupea harengus (larvae)	21380 ^d)	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Scophthalmus maximus	11220 ^d)	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Scophthalmus maximus	11482 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio	13400 ^{d)}	3	S	k1/k2 (total)	(Djomo et al., 1996)
	Pimephales promelas	6760	2	S	k1/k2 (parent)	(de Maagd, 1996)
Fluoranthene	Mollusca					
	Mytilus edulis	5920	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Mya arenaria	4120	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Fish					
	Pimephales promelas	3388	2	S	k1/k2 (parent)	(de Maagd, 1996)

Table 10: Bioaccumulation factors in fish and mollusca for the various PAHs (The Netherlands - Bureau REACH, 2009)

Table continues on next page

Substance	Species	BCF	Ra	Test	Type c)	References
Pyrene	Mollusca					
	Mya arenaria	6430	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Mytilus edulis	4430	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Dreissena polymorpha	16000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	Dreissena polymorpha	13000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	Dreissena polymorpha	35000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	Fish					
	Brachydanio rerio (eggs)	10000 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio (eggs)	30200 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio (larvae)	54954 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio (larvae)	53703 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Gadus morhua (larvae)	60256 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Gadus morhua (larvae)	85114 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Clupea harengus (larvae)	97724 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	Clupea harengus (larvae)	128825 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	Brachydanio rerio	4300	3	S	k1/k2 (total)	(Djomo et al., 1996)
	Poecilia reticulata	4810	3	S	k1/k2 (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	11300	2	R	equilibrium (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	2700	2	S	equilibrium (parent)	(de Voogt et al., 1991)
Dibenzofuran	Poecilia reticulata	3430	2		k1/k2 (parent)	(de Voogt et al., 1991)

Table continued from previous page

a) Reliability score: 1-reliable without restrictions, 2-reliable with restrictions, 3-unreliable, 4-not assignable; b) S: static exposure system, F: flow-through system, R: static renewal system; c) k1/k2: uptake rate/depuration rate, total: total compound concentration (including transformation products), parent: parent compound concentration, NS, not steady state; d) based on dry weights

4.3.2 Summary and discussion of bioaccumulation

The bioaccumulation potential of anthracene has been described in the Annex XV-Dossier for identifying anthracene as a SVHC. Anthracene has been placed on the Candidate List due to the identification as PBT-substance (European Chemicals Agency, 2008a).

Moreover, further constituents of anthracene oil show bioaccumulation potential, too. The BCF values of fluorene, dibenzofuran, phenanthrene, fluoranthene, and pyrene have shown to be >2000 in several studies. The last three constituents, additionally, fulfil the vB-criteria with BCFs >5000.

In summary, due to the properties of its constituents, anthracene oil fulfils the B and the vB criteria according to article 57 d) and e) of the REACH regulation.

5 HUMAN HEALTH HAZARD ASSESSMENT

Not relevant for this dossier

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

Not relevant for this dossier

7 ENVIRONMENTAL HAZARD ASSESSMENT

Anthracene oil consists of anthracene (>0.1 %) which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d). Moreover, fluorene, phenanthrene, and pyrene belong to the 16 US-EPA PAH for which the aquatic NOEC values are < 0.01 mg/L (The Netherlands - Bureau REACH, 2009).

7.1 Aquatic compartment

7.1.1 Toxicity test results

7.1.1.1 Fish

Short-term toxicity to fish

Long-term toxicity to fish

7.1.1.2 Aquatic invertebrates

- 7.1.1.3 Algae and aquatic plants
- 7.1.1.4 Sediment organisms
- 7.1.2 Other aquatic organismsCalculation of Predicted No Effect Concentration (PNEC)

7.1.2.1 PNEC water

- 7.1.2.2 PNEC sediment
- 7.2 Terrestrial compartment
- 7.2.1 Toxicity test results
- 7.2.1.1 Toxicity to soil macro organisms
- 7.2.1.2 Toxicity to terrestrial plants
- 7.2.1.3 Toxicity to soil micro-organisms
- 7.2.1.4 Toxicity to other terrestrial organisms

Toxicity to birds

Toxicity to other above ground organisms

8 PBT AND vPvB ASSESSMENT

8.1 Comparison with criteria from annex XIII

Anthracene oil is a UVCB substance consisting of a variety of different constituents. One main constituent is anthracene (3-25 %) which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d). Therefore also anthracene oil fulfils the PBT criteria according to Annex XIII of the REACH regulation.

Moreover, anthracene oil consists of further PAH, which are hardly degraded. Several studies show relatively long dissipation times for fluoranthene (DisDT₅₀ > 173 d), pyrene (DisDT₅₀ > 131 d), and carbazole (DegDT₅₀ > 184 d) in different soils (Grosser et al., 1991; Park et al., 1990). In a field study half-lives of 5.7 years for phenanthrene, 7.8 years for fluoranthene, and 8.5 years for pyrene have been measured in soil (Wild et al., 1991). Therefore, several constituents of anthracene-oil fulfil the P and/or the vP criteria according to Annex XIII of the REACH regulation.

In several studies conducted with different mollusc and fish species BCF values > 2000 were measured for fluorene, phenanthrene, fluoranthene, dibenzofuran and pyrene. For phenanthrene, pyrene and fluoranthene BCF values were even >5000 (Petersen and Kristensen, 1998; McLeese et al., 1987; Bruner et al., 1994; de Voogt et al., 1991; de Maagd, 1996; Djomo et al., 1996). This means that several constituents of anthracene oil meet the B and/ or vB criteria according to Annex XIII of the REACH regulation.

Fluorene, phenanthrene, anthracene and pyrene belong to the 16 US-EPA PAH for which the aquatic NOEC values are < 0.01 mg/L (The Netherlands - Bureau REACH, 2009). Therefore, anthracene oil also meets the T criterion.

8.2 Emission characterisation

8.3 Conclusions on the PBT and vPvB assessment

Anthracene oil is a UVCB substance consisting of a variety of different constituents. One main constituent is anthracene (3-25 %) which has already been identified as a PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d). Therefore, also anthracene oil fulfils the PBT criteria according to Annex XIII of the REACH regulation.

Phenanthrene, fluoranthene and pyrene are constituents of anthracene-oil (> 0.1%). These constituents of anthracene oil fulfil the PBT and the vPvB criteria. In summary, it can therefore be concluded that anthracene oil meets the P, vP, B, vB and T criteria and hence is considered a PBT and vPvB substance.

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

1 INFORMATION ON EXPOSURE

Anthracene oil is mainly used as an intermediate in the production of pure anthracene, which is intensively used in the production of artificial dyes. Anthracene oil is also used in the following applications:

- Component in technical tar oils (e.g. for production of carbon black, heating oils, bunker fuel)
- Production of basic chemicals
- Intermediate for phyto-pharmaceutical and human-pharmaceutical products.
- Impregnation agent (mostly as wood preservative, sometimes for ropes and sailcloth)
- Component in tar paints for special application (e.g. underwater corrosion protection)
- Component of waterproof membranes for roofing and other sealing purposes
- Component of asphalt used for road construction
- Supplementary blast furnace reducing agent
- Industrial viscosity modifier

For these applications the emission to the environment is estimated to be relevant. The emission factor for the life cycle steps "use" and "service life" and the related PECs can not be assessed for these applications, because these are wide dispersive uses and the emission factor also depends on the local environmental conditions. Though, there is no information on the annual amount of anthracene oil used for these environmentally relevant applications.

CEFIC was asked to answer detailed questions concerning exposure in January 2009. An official written reply to the questionnaire was received in July after the Annex XV dossier had already been supplied to ECHA. However, only information on main uses of anthracene oils was given.

2 INFORMATION ON ALTERNATIVES

2.1 Alternative substances

No information available.

2.2 Alternative techniques

No information available.

3 RISK-RELATED INFORMATION

Water Framework Directive (WFD)

According to Decision 2455/2001/EC anthracene and fluoranthene are on the priority list of the Water Framework Directive 2000/60/EC. Moreover, according to the latest common position adopted by the Council, they have been identified as a "priority hazardous substance" under the WFD, which means that cessation or phasing-out of discharges, emissions and losses of both has to be envisaged (Common position adopted by the Council of 29th November 2007, 11486/07). As a first step in this direction environmental quality standards for anthracene and fluoranthene are proposed in the common position: the annual average concentration of anthracene and fluoranthene should not exceed 0.1 μ g/l, while the maximum allowable concentration must not exceed 0.4 μ g/l in inland and other surface waters.

OTHER INFORMATION

It has to be mentioned that anthracene oil is only one example for a number of UVCB substances containing anthracene, irrespective from their origin (e.g. from chemical coal processing or from crude oil). Anthracene is a PBT-substance. Therefore all multi constituent substances and mixtures containing anthracene need to be considered for authorization in the future, since they also fulfil the PBT criteria according to Article 57 d) of the REACH-regulation. If those multi-constituent substances also contain further PAH, the vPvB criteria might be fulfilled, too.

References

Bruner KA, Fisher SW, Landrum PF. 1994. The role of the zebra mussel, Dreissenia polymorpha, on contaminant cycling: I.The effect of body size and lipid content on the bioconcentration of PCBs and PAHs. J Great Lakes Res 20(4):725-734.

Calvert JG, Atkinson JR, Becker KH, Kamens RM, Seinfeld JH, Wallington TJ, Yarwood G. 2002. The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons. Oxford University Press, Oxford.

Coover MP, Sims RC. 1987. The Effect of Temperature on Polycyclic Aromatic Hydrocarbon Persistence in an Unacclimated Agriculture Soil. Hazard Waste Hazard Mater 4(1).

de Maagd PG-J. 1996. Polycyclic aromatic hydrocarbons: Fate and effects in aquatic environment. Utrecht University, Utrecht, The Netherlands.

de Voogt P, van Hattum B, Leonards P, Klamer JC, Govers H. 1991 Sep. Bioconcentration of polycyclic heteroaromatic hydrocarbons in the guppy (Poecilia reticula). Aquat Toxicol 20(3):169-194.

Djomo JE, Garrigues P, Narbonne JF. 1996. Uptake and depuration of polycyclic aromatic hydrocarbons from sediment by the zebrafish (Brachydanio rerio). Environ Toxicol Chem 15(7):1177-1181.

European Chemicals Agency. 2008a. Candidate List.

European Chemicals Agency. 2008b. Chapter R.7a: Endpoint specific guidance. In: Guidance On Information Requirements And Chemical Safety Assessment. 1-428.

European Chemicals Agency. 2008c. R.16: Environmental exposure estimation. In: Guidance On Information Requirements And Chemical Safety Assessment. 1-138.

European Chemicals Agency. 2008d. Support document for identification of anthracene as a substance of very high concern. ECHA, 1-27.

European Commission. 2008. European risk assessment report, draft of April 2008, anthracene, CAS No: 120-12-7, EINECS No: 204-371-1.

Grosser RJ, Warshawsky D, Vestal JR. 1991. Indigenous and Enhanced Mineralization of Pyrene, Benzo[a]pyrene, and Carbazole in Soils. Am Soc Microbiol 57(12):3462-3469.

International Agency for Research on Cancer (IARC). 1985. Polynuclear aromatic Compounds, Part 4, Bitumens, Coal-tars and Derived Products, Shale Oils and Soots. IARC, Lyon, France.

Mackay D, Shiu WY, Ma K. 1992. Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals. Vol. II: Polynuclear aromatic hydrocarbons, polychlorinated dioxins and dibenzofurans. Lewis Publishers, Chelsea.

McLeese CW, Ray S, Burridge LE. 1987. Accumulation of polynuclear aromatic hydrocarbons by the clam Mya arenaria. Wastes in the Ocean, Vol 6 - Nearshore Waste Disposal 6:81-88.

MITI-List. 2002. Biodegradation and Bioaccumulation of Existing Chemical Substances under the Chemical Substance Control Law. National Institute of Technology and Evaluation, Japan.

Park KS, Sims RC, Dupont RR, Doucette WJ, Matthews JE. 1990 Feb. Fate of PAH compounds in two soil types: influence of volatilization, abiotic loss and biological activity. Environ Tox Chem 9(2):187-195.

Petersen GI, Kristensen P. 1998. Bioaccumulatoion of lipophilic substances in fish early life stages. Environ Toxicol Chem 17(7):1385-1395.

The Netherlands - Bureau REACH. 2009. Annex XV transitional report: coal tar pitch, high temperature (CTPHT).

Wild SR, Berrow ML, Jones KC. 1991. The persistence of polynuclear aromatic hydrocarbons (PAHs) in sewage sludge amended agricultural soils. Environ Pollut 72:141-157.

Wild SR, Jones KC. 1993. Biological and abiotic losses of polynuclear aromatic hydrocarbons (PAH) from soils freshly amended with sewage sludge. Environ Toxicol Chem 12:5-12.