2 December 2009

Substance name: **Anthracene oil**
EC number: **292-602-7**
CAS number: **90640-80-5**

MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF ANTHRACENE OIL AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS CMR, PBT AND vPvB PROPERTIES

Adopted on 2 December 2009

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TABLES

FOREWORD

Anthracene oil is an UVCB substance (substance of unknown or variable composition, complex reaction products or biological materials). It is characterised by a variable and high content of polycyclic aromatic hydrocarbons (PAHs) and heterocyclic compounds.

One relevant constituent present in anthracene oil in a concentration of 3-25 % is anthracene, which has been identified as a PBT-substance and has been placed on the Candidate List. Additionally other PAHs are present in anthracene oil in individual concentrations equal to or above 0.1% (weight/weight), such as phenanthrene, fluoranthene and pyrene.

The PBT and/or vPvB properties of the latter constituents have already been discussed in the Annex XV transitional report for coal tar pitch, high temperature and before in the Risk Assessment Report (RAR) for coal tar pitch, high temperature, indicating that the data have already been assessed for validity and relevance by a competent EU body. Therefore in the present document most data for individual PAH have been taken directly from the Annex XV transitional report and the RAR for coal tar pitch, high temperature. The data for anthracene are not discussed again in this support document, but references to the Anthracene Annex XV-Dossier are placed at appropriate positions in the text.

Substance Name: Anthracene oil

EC Number: 292-602-7

CAS Number: 90640-80-5

- *The substance is identified as a carcinogen according to Article 57 (a) of Regulation (EC) 1907/2006 (REACH).*
- *The substance is identified as a PBT according to Article 57 (d) of Regulation (EC) 1907/2006 (REACH).*
- *The substance is identified as a vPvB according to Article 57 (e) of Regulation (EC) 1907/2006 (REACH).*

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 (10-35%), fluoranthene (2-15%) and pyrene (1-10%). These three PAH fulfil the vPvB criteria, and fluoranthene and pyrene also fulfil the PBT criteria.

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

In addition, according to Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008[1] the classification as carcinogen (Carc. Cat.2, R45)[2] must be applied to anthracene oil unless it can be shown that the substance contains less than 0.005 % w/w benzo[a]pyrene (EINECS No 200-028-5).

Hence, anthracene oil is a substance meeting the criteria for identification as a carcinogen according Article 57(a) of the REACH Regulation where the conditions for its classification as a carcinogen set out in Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008 have been met.

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

Not available.

[1] Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

[2] This corresponds to a classification Carc. 1B; H350 in Annex VI, part 3, Table 3.1 of Regulation (EC) No 1272/2008.

JUSTIFICATION

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Chemical Name: Anthracene oil

EC Number: 292-602-7

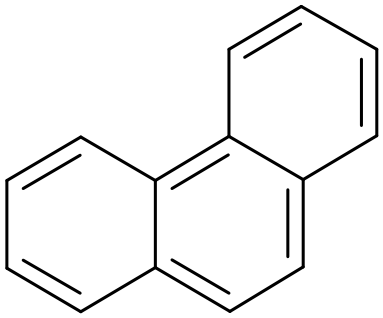
CAS Number: 90640-80-5

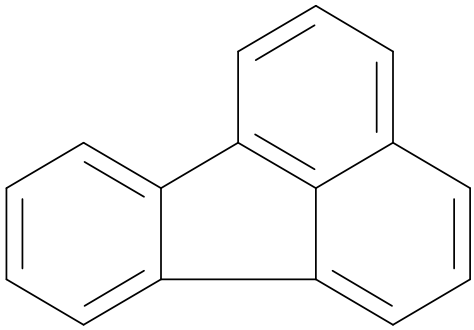
IUPAC Name:

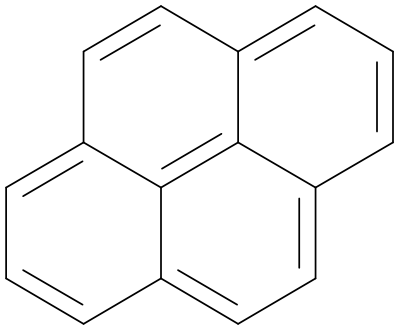
1.2 Composition of the substance

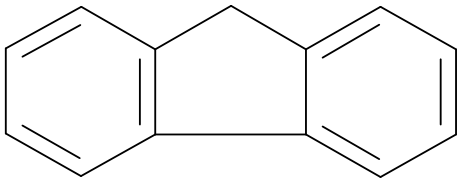
The anthracene oil derivates are complex and have variable compositions. Anthracene oil (CAS-No: 90640-80-5) is an UVCB substance consisting of three- to five-membered condensed aromatic hydrocarbons. Depending on the composition it is a solid or an oily liquid with a colour ranging from yellow over 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 process 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.

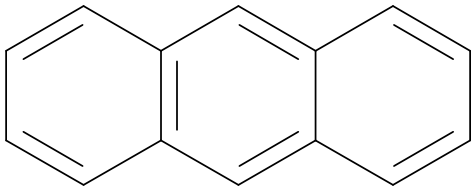
According to the EC inventory anthracene oil is a complex combination of polycyclic aromatic hydrocarbons obtained from coal tar having an approximate distillation range of 300°C to 400°C (572°F to 752°F). It is composed primarily of phenanthrene, anthracene and carbazole. The data provided by industry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

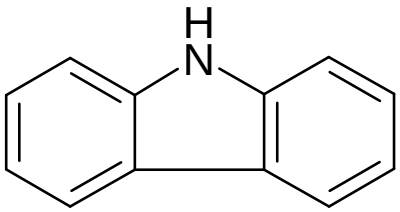
Chemical Name:	Phenanthrene
EC Number:	201-581-5
CAS Number:	85-01-8
IUPAC Name:	Phenanthrene
Molecular Formula:	C14H10
Structural Formula:	
Molecular Weight:	178.23
Typical concentration (% w/w):	
Concentration range (% w/w):	10 - 35

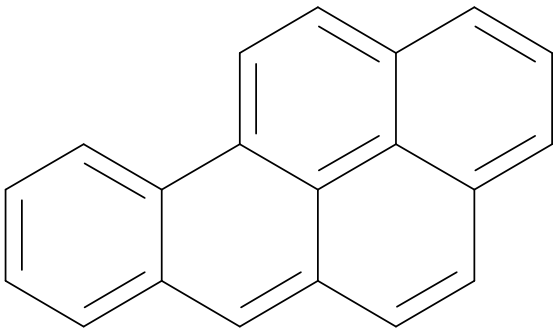
Chemical Name:	Fluoranthene
EC Number:	205-912-4
CAS Number:	206-44-0
IUPAC Name:	Fluoranthene
Molecular Formula:	C16H10
Structural Formula:	
Molecular Weight:	202.26
Typical concentration (% w/w):	
Concentration range (% w/w):	2 - 15

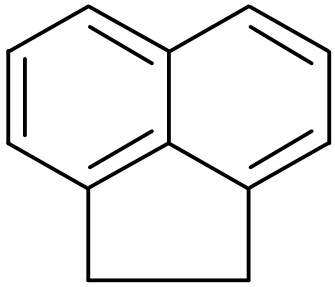
Chemical Name:	Pyrene
EC Number:	204-927-3
CAS Number:	129-00-0
IUPAC Name:	Pyrene
Molecular Formula:	C16H10
Structural Formula:	
Molecular Weight:	202.26
Typical concentration (% w/w):	
Concentration range (% w/w):	1 – 10

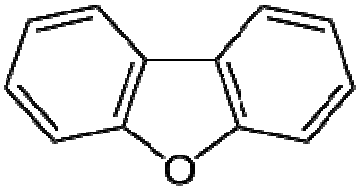
Chemical Name:	Fluorene
EC Number:	201-695-5
CAS Number:	86-73-7
IUPAC Name:	*9H*-fluorene
Molecular Formula:	C13H10
Structural Formula:	
Molecular Weight:	166.22
Typical concentration (% w/w):	
Concentration range (% w/w):	1 - 16

Chemical Name:	Anthracene
EC Number:	204-371-1
CAS Number:	120-12-7
IUPAC Name:	Anthracene
Molecular Formula:	C14H10
Structural Formula:	
Molecular Weight:	178.23
Typical concentration (% w/w):	
Concentration range (% w/w):	3 - 25

Chemical Name:	Carbazole
EC Number:	201-696-0
CAS Number:	86-74-8
IUPAC Name:	*9H*-carbazole
Molecular Formula:	C12H9N
Structural Formula:	
Molecular Weight:	167.21
Typical concentration (% w/w):	
Concentration range (% w/w):	1 – 10

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:	
Molecular Weight:	252.32
Typical concentration (% w/w):	< 0.05
Concentration range (% w/w):	

Chemical Name:	Acenaphthene
EC Number:	201-469-6
CAS Number:	83-32-9
IUPAC Name:	1,2 dihydroacenaphthylene
Molecular Formula:	C12H10
Structural Formula:	
Molecular Weight:	154.21
Typical concentration (% w/w):	
Concentration range (% w/w):	0.2 - 16

Chemical Name:	Dibenzofuran
EC Number:	205-071-3
CAS Number:	132-64-9
IUPAC Name:	Dibenzo[b,d]furan
Molecular Formula:	C12H8O
Structural Formula:	
Molecular Weight:	168,19
Typical concentration (% w/w):	
Concentration range (% w/w):	0.1-8

1.3 Physico-chemical properties

Table 1: Summary of physico-chemical properties of anthracene oil

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	3.84 – 5.20	IUCLID datafile; Depending on the concentration of the different substances

2 CLASSIFICATION AND LABELLING

2.1 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 support document 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	Notes
Anthracene oil	90640-80-5	648-079-00-6	Carc. Cat 2; R45	T; R45; S 53 – 45	HM
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; R50-53	T; N R: 45-46-60-61-43-50/53 S: 53-45-60-61	Carc. Cat. 2; R45: C ≥ 0.01 %

Notes:

H: *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.*

M: *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).*

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.

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.

Name	CAS-No	Index-No	Classification	Labelling	Notes
Anthracene oil	90640-80-5	648-079-00-6	Carc. Cat. 1B H350	GHS08 Dgr H350	HM
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	Carc. Cat. 2; R45: C ≥ 0.01 %

Notes:

H: *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.*

M: *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).*

3 ENVIRONMENTAL FATE PROPERTIES

3.1 Degradation

3.1.1 Stability

3.1.1.1 Phototransformation

Photolysis in the troposphere results in the formation of reactive hydroxyl (OH) and nitrate (NO_3) radicals and ozone (O_3), which react as oxidising agents with organic compounds like PAHs. Reactions with these radicals and ozone comprise the main degradation path of gas-phase PAH (Calvert et al., 2002). The atmospheric behaviour of the main constituents of anthracene oil[3] is shown below in Table 4.

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

PAH (number of rings)	Representative lifetime in air with respect to reaction with			
	OH		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 support document 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 only up to 3% of atmospheric anthracene has been observed to appear in particle phase (European Chemicals Agency, 2008d).

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

[3] 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) .

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 under simulated winter conditions.

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 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.

3.1.1.2 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. 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).

3.1.2 Biodegradation

3.1.2.1 Biodegradation estimation

The PAH listed in **Error! Reference source not found.** Table 5 were allocated to persistence classes on the basis of model calculations (Mackay et al., 1992). These half-lives were used 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 (The Netherlands - Bureau REACH, 2009)

Substance	Water		Soil		Sediment	
	class	Half-life [d]	class	Half-life [d]	class	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

3.1.2.2 Screening tests

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

Table 6: Biodegradation of several PAH according to the test method MITI I (OECD TG 301C).

Substance	BOD	Judgement
Phenanthrene	54 %	not readily biodegradable
Fluorene	0 %	not biodegradable
Carbazole	0 %	not biodegradable
Acenaphthene	0%	not biodegradable
Dibenzofuran	1%	not biodegradable

Coover and Sims tested the persistence of PAHs in an -unacclimated agricultural sandy loam soil in dependence on 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 elimination increased. 19% (2%) of phenanthrene, 71% (15%) of fluoranthene and 89% (43%) of pyrene were remaining at 20°C (30°C).

3.1.2.3 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 content 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 tested PAH are as follow: phenanthrene 83 – 193 days; fluoranthene 110 – 184 days; and pyrene 127 - 320 days. It has to be noted that the latter results were derived from a greenhouse study and should therefore not be used for the P-assessment. Various studies on PAH-contaminated soils have revealed 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 (European Commission, 2008; The Netherlands - Bureau REACH, 2009).

Grosser et al. (1991) studied the mineralisation of ^{14}C-labelled pyrene and carbazole in three different soils. The mineralisation 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 mineralisation degree of pyrene was calculated between 10% and 48% and for carbazole between undetectable and 46% within the test duration.

The fate of several PAHs in two different soils was tested by 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).

Table 7: Half-lives for PAHs in soil (of relevant constituents of anthracene oil)

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: $DisDT_{50}$ = 27 – 53 d $DisDT_{50}$ = 13 – 18 d	(Park et al., 1990)
Fluoranthene	$DisDT_{50}$ =7.8 years (field study)	(Wild et al., 1991)
	$DisDT_{50}$ =110 – 184 d (microcosm study)	(Wild and Jones, 1993)
	Elimination half- life in two different soils: $DisDT_{50}$ = 173 – 630 d $DisDT_{50}$ = 277 – 578 d	(Park et al., 1990)
Pyrene	Degradation half-life: $DegDT_{50}$ > 184 d (10 – 48% mineralisation 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: $DisDT_{50}$ = 131 – 408 d $DisDT_{50}$ = 193 – 408 d	(Park et al., 1990)
Carbazole	Degradation half-life: $DegDT_{50}$ > 184 d (undetectable – 46% mineralisation in 184 d)	(Grosser et al., 1991)

3.1.3 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 not readily biodegradable PAH constituents. Model calculations by Mackay et al. (1992) indicate that acenaphtene, fluorene, phenanthrene, fluoranthene, and pyrene show a half-life in sediment of more than 180 days.

Screening studies (OECD TG 301C) revealed, that phenanthrene, acenaphtene, fluorene, carbazole, and dibenzofuran as representative constituents of anthracene oil are not readily biodegradable (MITI-List, 2002).

Further studies showed relatively long dissipation times for fluoranthene ($DisDT_{50}$ > 173 d), pyrene ($DisDT_{50}$ > 131 d), and carbazole ($DegDT_{50}$ > 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 were measured in soil (Wild et al., 1991).

Hence, several constituents of anthracene oil fulfil the P and/or the vP criteria according to Annex XIII of the REACH regulation.

3.2 Environmental distribution

3.2.1 Adsorption/desorption

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

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

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

a) Values were 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.

3.2.2 Volatilisation

For the substance anthracene oil no measured data are available at the moment. According to the constituents' Henry's Law constants anthracene oil is expected 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).

3.2.3 Distribution modelling

For the main constituents of anthracene oil the behaviour in the wastewater treatment plant was calculated under the assumption that no biodegradation occured (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] (Pa*m³/mol)	Distribution of PAH in STP[b]			
		% 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
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

[a] calculation 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.

3.3 Bioaccumulation

3.3.1 Aquatic bioaccumulation

3.3.1.1 Bioaccumulation estimation

Based on the substance's log K_{OW} range from 3.84 to 5.20 constituents of anthracene oil are expected to bioaccumulate.

3.3.1.2 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 Voogt et al., 1991; Djomo et al., 1996; de Maagd, 1996) and in the Annex XV transitional report for coal tar pitch, high temperature (McLeese et al., 1987). The most relevant studies and results are summarised in Table 10.

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

Substance	Species	BCF	R[a)]	Test system [b)]	Type [c)]	References
Fluorene	***Fish***					
	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	***Mollusca***					
	Mytilus edulis	1240	1	F	k1/k2 (parent)	(McLeese et al., 1987)
	Mya arenaria	1280	1	F	k1/k2 (parent)	(McLeese et al., 1987)
	Fish					
	Cyprinodon variegatus	810[d)]	1	F	k1/k2 (parent)	(Jonsson et al., 2004)
	Cyprinodon variegatus	2229[e)]	1	F	k1/k2 (parent)	(Jonsson et al., 2004)
	Cyprinodon variegatus	700[d)]	1	F	equilibrium (parent)	(Jonsson et al., 2004)
	Cyprinodon variegatus	1623[e)]	1	F	equilibrium (parent)	(Jonsson et al., 2004)
	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)
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					
	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)

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) low exposure concentrations; e) high exposure concentrations.

3.3.2 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, several constituents of anthracene oil fulfil the B and the vB criteria according to Annex XIII of the REACH regulation.

4 HUMAN HEALTH HAZARD ASSESSMENT

Not considered in this document..

5 ENVIRONMENTAL HAZARD ASSESSMENT

5.1 Aquatic compartment

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). Therefore, the toxicity data are not presented here, again. Fluoranthene and pyrene, which are also present in anthracene oil are also toxic to aquatic organisms.

Exposure to PAH (such as anthracene, fluoranthene and pyrene) under UV-radiation enhances the ecotoxicity of several PAH, i.a., in fish, invertebrates and algae (The Netherlands - Bureau REACH, 2009). The mechanism of photo-enhanced toxicity is not fully understood. Enhanced effects have been attained already with very short exposures to natural sunlight or UV-light (0.5 to 6 hours) and with light intensities corresponding to conditions in several meters depth of natural water. Hence, photo-enhanced toxicity is considered a relevant phenomenon in the environment.

The most reliable study with the most sensitive organism for the evaluation of the toxicity of fluoranthene was published by Spehar et al. (1999). It has been shown that ultraviolet (UV) light increases the acute toxicity of fluoranthene (Spehar et al., 1999). For pyrene two studies as an example for the toxicity were selected and described in the following tables (Lyons et al. 2002; Pelletier et al. 1997).

Available studies on the toxicity to fish, invertebrates and algae were described in detail in the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009). The most reliable acute and chronic toxicity data on fish, invertebrates and algae are listed in Tables 11 to 15.

5.1.1 Toxicity test results

5.1.1.1 Fish

Short-term toxicity to fish

Table 11 Examples for acute toxicity of fluoranthene to fish species.

Substance	Species	Exposure duration	End-point	Effect	Conc. (mg/L)	Ref.
Fluoranthene	*Pseudopleuronectes Americanus* (winter flounder)	96 h	LC_{50}	Mortality	0.0001*	(Spehar et al., 1999)
	Pseudopleuronectes americanus (winter flounder)	96 h	LC_{50}	Mortality	> 0.188#	(Spehar et al., 1999)

*UV light exposure; # fluorescent light

Acute toxicity data for pyrene on fish are currently not available.

Long-term toxicity to fish

Table 12: Examples for chronic toxicity of fluoranthene to fish species. Data were taken from the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Substance	Species	Exposure duration	End-point	Effect	Conc. (mg/L)	Ref.
Fluoranthene	*Pimephales promelas*	32 d	NOEC	ELS	0.0014	(Spehar et al., 1999)
	Pimephales promelas	11w	NOEC	Survival of hatchlings	< 0.0062	(Diamond et al., 1995)

Chronic toxicity data for pyrene on fish are currently not available.

5.1.1.2 Aquatic invertebrates

Short-term toxicity to aquatic invertebrates

Table 13 Short-term toxicity to aquatic invertebrates

Substance	Species	Exposure duration	End-point	Effect	Conc. (mg/L)	Ref.
Fluoranthene	*Americamysis bahia* (reported as *Mysidopsis bahia*)	96 h	LC50	Mortality	0.0014 *	(Spehar et al., 1999)
	Americamysis bahia (reported as *Mysidopsis bahia*)	96 h	LC50	Mortality	0.031[#]	(Spehar et al., 1999)
Pyrene	*Mulinia lateralis* (Dwarf Surf Clam)	48 h	EC50	Bivalve embryo response	0.00023*	(Pelletier et al., 1997)
	Mulinia lateralis (Dwarf Surf Clam)	96 h	LC50	Mortality	0.00168*	(Pelletier et al., 1997)
	Crassostrea gigas (Pacific oyster)	48 h	NOEC	Developmental success	0.0005 *	(Lyons et al., 2002)

*UV light exposure; [#] fluorescent light; [a] bivalve embryo response: Embryo/larval bivalve survival and development were determined by counting the number of normal larvae per millilitre in each replicate. Bivalve embryo/ larval survival and development are later referred to as bivalve embryo response.

Long-term toxicity to aquatic invertebrates

Table 14: Examples for chronic toxicity of pyrene and fluoranthene to aquatic invertebrates. Data were taken from the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Substance	Species	Exposure duration	End-point	Effect	Conc. (mg/L)	Ref.
Pyrene	*Crassostrea gigas*	48 h	NOEC	Shell development	0.0005 *	(Lyons et al., 2002)
	Ceriodaphnia dubia	7 d	EC10	Reproduction	0.0021	(Bisson et al., 2000)
Fluoranthene	*Mysidopsis bahia*	31 d	NOEC	Reproduction	0.0006 *	(Spehar et al., 1999)
	Daphnia magna	21 d	NOEC	Growth	0.0014 *	(Spehar et al., 1999)

*UV light exposure

5.1.1.3 Algae and aquatic plants

Table 15: Examples for chronic toxicity of pyrene and fluoranthene to algae and aquatic plants. Data were taken from the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Substance	Species	Exposure duration	End-point	Effect	Conc. (mg/L)	Ref.
Pyrene	*Pseudokirchneriella subcapitata*	72 h	EC10	Growth	0.0012	(Bisson et al., 2000)
Fluoranthene	*Pseudokirchneriella subcapitata*	72 h	EC10	Growth	0.0086	(Bisson et al., 2000)

6 PBT AND vPvB ASSESSMENT

6.1 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 anthracene oil also fulfils the PBT criteria according to Annex XIII of the REACH regulation.

Moreover, anthracene oil consists of further PAH, which also fulfil the criteria of Annex XIII.

Fluoranthene:

In a field study a half-live of 7.8 years for fluoranthene has been measured in soil (Wild et al., 1991). Several other studies show relatively long dissipation times for fluoranthene ($DisDT_{50}$ > 173 d) in different soils (Park et al., 1990; Grosser et al., 1991). Therefore, the P and the vP criteria are fulfilled.

In studies conducted with different mollusc and fish species BCF values > 5000 (3388 to 5920) have been measured (McLeese et Burridge, 1987 de Maagd, 1996). This means that the B and the vB criteria are fulfilled, too.

Additionally, the long-term aquatic NOECs of fluoranthene are in the range from 0.0014 to 0.0006 mg/l (Spehar et al., 1999). Therefore also the T criterion is fulfilled.

Pyrene:

In a field study a half-live of 8.5 years for pyrene has been measured in soil (Wild et al., 1991). Several other studies show relatively long dissipation times for pyrene ($DisDT_{50}$ > 131 d) in different soils (Park et al., 1990; Grosser et al., 1991). Therefore, the P and the vP criteria are fulfilled.

In several studies conducted with different mollusc and fish species BCF values > 5000 were measured (McLeese et Burridge, 1987; de Voogt et al., 1991). This means both the B and the vB criteria are fulfilled, too.

Additionally, the aquatic NOECs of pyrene are below 0,01 mg/l. Chronic values for fish are not available, but NOECs fo aquatic invertebrates are as low as 0.0005 mg/l (shell development, *Crassostrea gigas*, Lyons et al., 2002). Therefore also the T criterion is fulfilled.

Phenanthrene:

In a field study a half-live of 5.7 year for phenanthrene, has been measured in soil (Wild et al., 1991). Therefore, the P and the vP criteria are fulfilled.

In one study conducted with fish (Pimephales promelas) a BCF value > 5000 was measured (de Maagd, 1996). This means that the B and the vB criteria are fulfilled, too.

6.2 Summary and overall conclusions on the PBT, vPvB or equivalent level of concern properties

In accordance with the guidance available for assessment of multi-constituent and UVCB substances, the PBT assessment for anthracene oil focuses on the assessment of its PAH-constituents

present in concentrations ≥ 0.1%[4] such as anthracene (presence 3-25%), fluoranthene (2-15%), pyrene (1-10%) and phenanthrene (10-35%).

An overview on the conclusions drawn on persistence, potential for bioaccumulation and toxicity to human health and/or the environment based on comparison of the data presented for four indicator PAH-constituents of anthracene oil with the PBT/vPvB criteria of Annex XIII of the REACH Regulation is provided in Table 16.

Table 16: Overview on conclusions on fulfilment of the (v)P-, (v)B- or T-criteria of Annex XIII of the REACH Regulation for the four indicator PAH-constituents of anthracene oil

Substance	Persistence	Bioaccu-mulation	Toxicity Human health	Toxicity Aquatic Environment	Conclusion
Anthracene	vP	B	-	T	PBT
Phenanthrene	vP	vB	-	-	vPvB
Fluoranthene	vP	vB	-	T	PBT/vPvB
Pyrene	vP	vB	-	T	PBT/vPvB

Based on the data available, it is concluded that two PAH-constituents present in anthracene oil in concentrations equal to or above 0.1% are to be considered as both vPvB and PBT substances. These are fluoranthene and pyrene.

Phenanthrene fulfils the vPvB criteria, but not the PBT criteria. Anthracene fulfils the PBT criteria, but not the vPvB criteria.

In summary, anthracene oil needs to be considered as a substance with both vPvB and PBT properties because of the above conclusions on the vPvB and PBT properties of its constituents anthracene, fluoranthene, pyrene and phenanthrene. It is concluded that anthracene oil is a substance containing at least 16% of PAH constituents with vPvB and/or PBT properties.

[4] Chapter R.11 (PBT assessment) of the guidance on information requirements and chemical safety assessment (ECHA)

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