



4 December 2009

Substance name: Anthracene oil, anthracene paste
EC number: 292-603-2
CAS number: 90640-81-6

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

Adopted on 4 December 2009

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FOREWORD

Anthracene oil, anthracene paste 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, anthracene paste in a concentration of 15-50% 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, anthracene paste in individual concentrations equal to or above 0.1% (weight/weight), such as phenanthrene.

The vPvB properties of the latter constituent have been discussed already 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. In the present document the data for individual PAH have therefore been taken mostly 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 given at the relevant place in the text.

Substance Name: Anthracene oil, anthracene paste

EC Number: 292-603-2

CAS Number: 90640-81-6

- *The substance is identified as a carcinogen (category 2, R45) according to Article 57 (a) of Regulation (EC) 1907/2006 (REACH).*
- *The substance is identified as a mutagen (category 2, R46) according to Article 57 (b) 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, anthracene paste is a UVCB substance consisting of different constituents, among them various PAH. One relevant constituent is anthracene which is present in anthracene oil, anthracene paste in the range of 15-50 %. Anthracene has been placed on the Candidate List due to the identification as a PBT-substance. Moreover, anthracene oil, anthracene paste consists of further PAH in concentrations above 0.1% (w/w). One constituent, phenanthrene (5-30%), fulfils the vPvB criteria.

Hence, anthracene oil, anthracene paste, fulfils the PBT and the vPvB-criteria according Article 57 d) and e) of the REACH regulation.

According to Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008¹ the classification as carcinogen (Carc. Cat.2, R45)² must be applied to anthracene oil, anthracene paste unless it can be shown that the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7) and less than 0.005 % w/w benzo[a]pyrene (EINECS No 200-028-5).

Pursuant to Annex IV of Commission Regulation (EC) No 790/2009³ as of 1 December 2010 the classification as mutagen (Muta. Cat.2; R46) must be applied to anthracene oil, anthracene paste unless the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7).⁴

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.

³ Commission Regulation (EC) No 790/2009 of 10 August 2009 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures (1st ATP)

⁴ Pursuant to the 1st ATP, the classification according to Table 3.1 of Annex VI, part 3, of Regulation (EC) No 1272/2008 will as of 1 December 2010 be mutagen category 1B, H340.

Hence, anthracene oil, anthracene paste is a substance meeting the criteria for identification as a carcinogen and mutagen according to Article 57(a) and 57 (b) of the REACH Regulation where the conditions for its classification have been met.

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

Not available.

JUSTIFICATION

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Chemical Name: Anthracene oil, anthracene paste

EC Number: 292-603-2

CAS Number: 90640-81-6

IUPAC Name:

1.2 Composition of the substance

The anthracene oil, anthracene paste derivatives are complex and have variable compositions. According to the EC inventory: the anthracene-rich solid (EC No. 292-603-2) is obtained by the crystallization and centrifuging of anthracene oil. It is composed primarily of anthracene, carbazole and phenanthrene. The concentration range reported in the following refers to the data provided by industry in the IUCLID 5 files.

The most relevant compounds are listed below:

Chemical Name: Anthracene

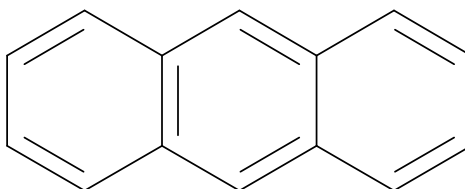
EC Number: 204-371-1

CAS Number: 120-12-7

IUPAC Name: Anthracene

Molecular Formula: C₁₄H₁₀

Structural Formula:

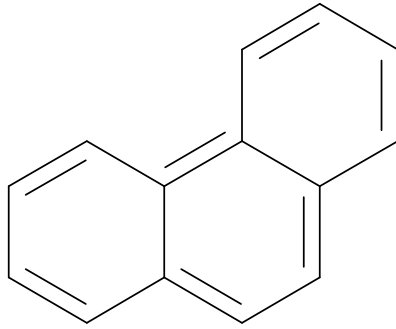


Molecular Weight: 178.23

Typical concentration (% w/w):

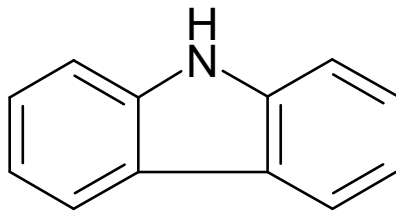
Concentration range (% w/w): 15-50

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): 5-30

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): 5-30

1.3 Physico-chemical properties

Table 1: Summary of physico-chemical properties of anthracene oil, anthracene paste (CAS Number 90640-81-6)

REACH ref Annex, §	Property	IUCLID section	Value	
VII, 7.1	Physical state at 20°C and 101.3 kPa	4.1	solid	IUCLID data file
VII, 7.2	Melting/freezing point	4.2	120-200 °C	IUCLID datafile; depending on the concentration of the different substances
VII, 7.3	Boiling point	4.3	300-350 °C (at 1013.25 Pa)	IUCLID datafile; depending on the concentration of the different substances
VII, 7.5	Vapour pressure	4.6	$9.4 \cdot 10^{-4}$ - 0.091 Pa (at 20 °C)	IUCLID datafile; depending on the concentration of the different substances
VII, 7.7	Water solubility	4.8	0.047 - 1.6 mg/L (at 25 °C)	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 - 4.68 (at 25 °C)	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, anthracene paste has index number 648-103-00-5 in Annex VI, part 3, Tables 3.1 and 3.2 of Regulation (EC) No 1272/2008⁵.

Its classification has been updated under the same index number in Annex IV of Commission Regulation (EC) No 790/2009⁶. Classification as mutagen (Muta. Cat.2; R 46) has been added.

Pursuant to Annex IV of Commission Regulation (EC) No 790/2009 anthracene oil, anthracene paste will as of 1 December 2010 be listed in Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Annex VI, part 3, of Regulation (EC) No 1272/2008 as shown in Table 2.

Table 2: Classification and labelling of anthracene oil, anthracene paste according to Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008 as of 1 December 2010.

Name	CAS-No	Index-No	Classification	Labelling	Notes
Anthracene oil, anthracene paste	90640-81-6	648-103-00-5	Carc. Cat. 2; R45 Muta. Cat.2; R46	T; R45-46; S 53 – 45	HJM

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.

J: The classification as a carcinogen or mutagen need not apply if it can be shown that the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7).

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, anthracene paste as hazardous substance according to Regulation (EC) No 1272/2008 (Annex VI, part 3, Table 3.1 (the list of harmonised classification and labelling of hazardous substances)) as of 1 December 2010 is provided in Table 3.

⁵ 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.

⁶ Commission Regulation (EC) No 790/2009 of 10 August 2009 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures (1st ATP)

Table 3: Classification and labelling of anthracene oil, anthracene paste according to Annex VI, part 3, Table 3.1 of Regulation (EC) No 1272/2008 as of 1 December 2010 .

Name	Cas-No	Index-No	Classification	Labelling	Notes
Anthracene oil, anthracene paste	90640-81-6	648-103-00-5	Carc. Cat. 1B H350 Muta. Cat. 1B H340	GHS08 Dgr H350 H340	HJM

Notes:

H: 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 for manufacturers, importers or downstream users of this substance apply to all other hazard classes and categories. For hazard classes where the route of exposure or the nature of the effects leads to a differentiation of the classification of the hazard class, the manufacturer, importer or downstream user is required to consider the routes of exposure or the nature of the effects not already considered.

J: The classification as a carcinogen or mutagen need not apply if it can be shown that the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7).

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 (NO₃) radicals and ozone (O₃), which react as oxidizing agent with organic compounds, like PAHs. These radical and ozone reactions comprise main the degradation path of gas-phase PAH (Calvert et al., 2002). The atmospheric behaviour of the main constituents of anthracene oil, anthracene paste⁷ is shown below in Table 4.

Table 4: Phototransformation of the relevant constituents present in anthracene oil, anthracene paste. Data are 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	-	-
Carbazole (2) ^{a)}	9.6 h	-	-	-

a) Especially calculated for this support document with AOPwin v1.91

For these substances the transformation rate in 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).

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 under simulated winter conditions.

Environmentally relevant exposure occurs in the whole water column and, in the case of anthracene oil, anthracene paste, especially in sediment and soil. Photodegradation of anthracene oil, anthracene paste 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 in the environment.

3.1.1.2 Hydrolysis

⁷ Please note that the data relevant for the constituent anthracene are not shown in this document, since anthracene has already been identified as a PBT substance (European Chemicals Agency, 2008d)

Hydrolysis as a way of abiotic degradation can be considered as not relevant for the main substances of the constituents 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, anthracene paste constituents can be made.

3.1.2 Biodegradation

3.1.2.1 Biodegradation estimation

The PAH listed in the Table5 below were allocated on the basis of model calculations (Mackay et al., 1992). These half-lives were applied in the Annex XV transitional report of coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Table 5: Half-life classes of phenanthrene (The Netherlands - Bureau REACH, 2009)

Substance	Water		Soil		Sediment	
	class	Half-life [d]	class	Half-life [d]	class	Half-life [d]
Phenanthrene	4	13 – 42	6	125 – 420	7	420 – 1250

3.1.2.2 Screening tests

In a 28 day ready biodegradability test (MITI I, OECD 301C) using 100 mg l⁻¹ PAH, respectively, and 30 mg l⁻¹ sludge no ready biodegradation was detected for phenanthrene (54% BOD) and carbazole (0% BOD) (MITI-List, 2002).

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 was remaining. With increasing temperature the elimination increased to 19% (2%) of remaining phenanthrene, 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 an elimination half-life of 5.7 years for phenanthrene. 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 phenanthrene were 83 – 193 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 (The Netherlands - Bureau REACH, 2009)

Grosser et al. studied the mineralization of ¹⁴C-labeled carbazole in three different soils (Grosser et al., 1991). 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 of carbazole was measured 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 in the range of 27 and 53 days (second soil: 13 – 18 days).

Table 6: Half-lives of relevant compounds present in anthracene oil, anthracene paste

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)
	DisDT ₅₀ = 8.5 years (field study)	(Wild et al., 1991)
Carbazole	Degradation half-life: DegDT ₅₀ > 184 d (undetectable – 46% mineralization in 184 d)	

3.1.3 Summary and discussion of persistence

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

Moreover, anthracene oil, anthracene paste consists of further hardly degradable PAHs. The model calculations by Mackay et al. (1992) indicate that phenanthrene show half-times in sediment of more than > 180 days.

Screening studies (OECD TG 301C) revealed, that phenanthrene and carbazole are not readily biodegradable (MITI-List, 2002). Further studies showed relatively long dissipation times for carbazole (DegDT₅₀ > 184 d) (Grosser et al., 1991).

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

Hence, two constituents of anthracene oil, anthracene paste fulfil the P and 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 $\log K_{OC} = 0.81 * \log K_{OW} + 0.10$ (European Chemicals Agency, 2008b). The results are shown below in Table 7.

Table 7: $\log K_{OW}$ and $\log K_{OC}$ data of the relevant constituents present in anthracene oil, anthracene paste

Substance	CAS-No.	$\log K_{OW}$ ^{a)}	$\log K_{OC}$	K_{OC} (l/kg) ^{b)}
Phenanthrene	85-01-8	4.57	3.80	6,309
Carbazole	86-74-8	3.84	3.21	1,621

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, anthracene paste 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, anthracene paste no measured data are available at the moment. According to the constituent's Henry's Law constants anthracene oil, anthracene paste is expected to be moderately volatile. The calculated values are shown in Table 8 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 components of anthracene oil, anthracene paste 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 8.

Table 8: Henry constants and volatilisation of main constituents in municipal waste water treatment plants.

Substance	Henry-constant ^a (Pa*m ³ /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
Carbazole	0.01	0.0	83.3	16.7	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, anthracene paste constituents depends on the composition of the oil. Nevertheless volatilisation is not considered as a relevant route of distribution for anthracene oil, anthracene paste.

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 4.68, anthracene oil, anthracene paste is 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; Bruner et al., 1994; Petersen and Kristensen, 1998). The most relevant studies and results are summarized in the following Table 9.

Table 9: Bioaccumulation factors in fish for phenanthrene (The Netherlands - Bureau REACH, 2009)

Substance	Species	BCF	R ^{a)}	Test system ^{b)}	Type ^{c)}	References
Phenanthrene	<i>Mollusca</i>					
	<i>Mytilus edulis</i>	1240	1	F	k1/k2	(McLeese et al., 1987)
	<i>Mya arenaria</i>	1280	1	F	k1/k2	(McLeese et al., 1987)
	<i>Fish</i>					
	<i>Cyprinodon variegatus</i>	810 ^{d)}	1	F	k1/k2 (parent)	(Jonsson et al., 2004)
	<i>Cyprinodon variegatus</i>	2229 ^{e)}	1	F	k1/k2 (parent)	(Jonsson et al., 2004)
	<i>Cyprinodon variegatus</i>	700 ^{d)}	1	F	equilibrium (parent)	(Jonsson et al., 2004)
	<i>Cyprinodon variegatus</i>	1623 ^{e)}	1	F	equilibrium (parent)	(Jonsson et al., 2004)
<i>Pimephales promelas</i>	6760	2	S	k1/k2 (parent)	(de Maagd, 1996)	

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 Terrestrial bioaccumulation

3.3.3 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, anthracene paste show bioaccumulative potential, too. The BCF of phenanthrene resulted in values >5000 in one study.

In summary, two constituents of anthracene oil, anthracene paste fulfils the B and/or 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, anthracene paste 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). The toxicity data are not presented here again.

5.1.1 Toxicity test results

5.1.1.1 Fish

Short-term toxicity to fish

Long-term toxicity to fish

5.1.1.2 Aquatic invertebrates

Short-term toxicity to aquatic invertebrates

Long-term toxicity to aquatic invertebrates

5.1.1.3 Algae and aquatic plants

5.1.1.4 Sediment organisms

5.1.1.5 Other aquatic organisms

5.1.2 Calculation of Predicted No Effect Concentration (PNEC)

5.1.2.1 PNEC water

5.1.2.2 PNEC sediment

5.2 Terrestrial compartment

5.2.1 Toxicity test results

5.2.1.1 Toxicity to soil macro organisms

5.2.1.2 Toxicity to terrestrial plants

5.2.1.3 Toxicity to soil micro-organisms

5.2.1.4 Toxicity to other terrestrial organisms

Toxicity to birds

Toxicity to other above ground organisms

5.2.2 Calculation of Predicted No Effect Concentration (PNEC_{soil})

5.3 Atmospheric compartment

5.4 Microbiological activity in sewage treatment systems

5.4.1 Toxicity to aquatic micro-organisms

5.4.2 PNEC for sewage treatment plant

5.5 Calculation of Predicted No Effect Concentration for secondary poisoning (PNEC_{oral})

5.6 Conclusion on the environmental classification and labelling

6 PBT AND VPVB ASSESSMENT

6.1 Comparison with criteria from annex XIII

Anthracene oil, anthracene paste is a UVCB substance consisting of a variety of different constituents. One main constituent is anthracene (15-50 %) which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d). Therefore also anthracene oil, anthracene paste fulfils the PBT criteria according to Annex XIII of the REACH regulation.

Moreover, a constituent of anthracene oil, anthracene paste is phenanthrene (5-30%) which also fulfils the criteria of Annex XIII:

In a field study a half-life of 5.7 years 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, anthracene paste focuses on the assessment of its PAH-constituents present in concentrations $\geq 0.1\%$ ⁸ such as anthracene (15-50%) and phenanthrene (5-30%).

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 two indicator PAH-constituents of anthracene oil, anthracene paste with the PBT/vPvB criteria of Annex XIII of the REACH Regulation is provided in Table 10.

Table 10: Overview on conclusions on fulfilment of the (v)P-, (v)B- or T-criteria of Annex XIII of the REACH Regulation for the two indicator PAH-constituents of anthracene oil, anthracene paste					
Substance	Persistence	Bioaccumulation	Toxicity Human health	Toxicity Aquatic Environment	Conclusion
Anthracene	vP	B	-	T	PBT
Phenanthrene	vP	vB	-	-	vPvB

Based on the data available, it is concluded that

- phenanthrene fulfils the vPvB criteria, but not the PBT criteria

⁸ Chapter R.11 (PBT assessment) of the guidance on information requirements and chemical safety assessment (ECHA)

- anthracene fulfils the PBT criteria, but not the vPvB criteria.

In summary, anthracene oil, anthracene paste 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 and phenanthrene. It is concluded that anthracene oil, anthracene paste is a substance containing at least 20% of PAH-constituents with vPvB or PBT properties.

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.
- 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.
- Jonsson G, Bechmann RK, Bamber SD, Baussant T. 2004. Bioconcentration, biotransformation, and elimination of polycyclic aromatic hydrocarbons in sheepshead minnows (*Cyprinodon variegatus*) exposed to contaminated seawater. *etc* 23(6):1538-1548.
- 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, Burrige 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. Bioaccumulation 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.