TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

Substance name: Extracts (petroleum), heavy paraffin distillate solvent

EC number: 265-103-7

CAS number: 64742-04-7

Molecular formula: Not applicable

Structural formula: Not applicable

Summary of the evaluation:

The substance, extracts (petroleum) heavy paraffin distillate solvent, is a complex combination of hydrocarbons obtained as the extract from a solvent extraction process. It consists predominantly of aromatic hydrocarbons having carbon numbers predominantly in the range of C20 through C50. This stream is likely to contain 5 wt. % or more of 4- to 6-membered condensed ring aromatic hydrocarbons. Petroleum substances can be regarded within REACH as substances of "Unknown or Variable composition, Complex reaction products or Biological materials" ("UVCBs").

Extracts (petroleum) heavy paraffin distillate solvent is considered as a PBT/vPvB substance based on screening data. However, no final conclusion on the PBT/vPvB-status of the substance was drawn in the TC NES Subgroup. Further PBT cathegorisation of the UVCB-substance is dependent on guidance development for substances containing PBT or vPvB constituents. Provisionally, extracts (petroleum) heavy paraffin distillate solvent can be regarded as a substance with PBT/vPvB impurities.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name:	Extracts (petroleum), heavy paraffin distillate solvent
EC Number:	265-103-7
CAS Number:	64742-04-7
IUPAC Name:	
Molecular Formula:	Not applicable
Structural Formula:	Not applicable
Molecular Weight:	Not applicable
Synonyms:	600 N Extract Aromatic extract DAE, distillate extract, distillate aromatic extract E40 Extract (heavy) Heavy paraffinic distillate FEU Extract HNE (Heavy neutral distillate extract Hydrocarbons C20-C50 PDU/FEU/MDU Extract Probor 80

1.1 Purity/Impurities/Additives

The substance belongs to UVCB-substances. According to the producers, the substance consists of:

- Saturated HCs : 10 - 20%
- Aromatic HCs : 60 - 80%
- Polar HCs : 10 - 20%

Analysis of individual PAHs in a sample used as test substance in two ecotoxicity studies (BP, 1994a and 1995) are presented in Table 1.2. Eight of these substances are included in the EU risk assessment of coal tar pitch, high temperature (CAS 65996-93-2; European Commission, 2007).

Table 1.2 Polyaromatic hyrdocarbons found to be present in the substance.

	Concentration	Included in the RAR of coal tar pitch, high temperature (x)
Fluoranthene	0.7 mg/kg	X
Pyrene	2.5 mg/kg	X
Benz(a)anthracene	2.6 mg/kg	X
Chrysene/Tiphenylene	27 mg/kg	X
Benzofluoranthenes	23 mg/kg	X
Benzo(e)pyrene	28 mg/kg	
Benzo(a)pyrene	6.4 mg/kg	X

Perylene	5.1 mg/kg	
Dibenz(a,j)anthracene	1.5 mg/kg	
Dibenz(a,h)anthracene	3.4 mg/kg	X
Indeno(1,2,3-cd)pyrene	10 mg/kg	X
Benzo(g,h,i)perylene	26 mg/kg	

However, it is noted, that the consistence is variable.

The substance has the following description in EINECS: "A complex combination of hydrocarbons obtained as the extract from a solvent extraction process. It consists predominantly of aromatic hydrocarbons having carbon numbers predominantly in the range of C20 through C50. This stream is likely to contain 5 % w/w or more of 4- to 6-membered condensed ring aromatic hydrocarbons"

Information from the producers describes the composition by carbon numbers C13-C55, primarily of aromatic hydrocarbons, alkylbenzenes, polycyclic aromatic compounds, cycloalkanes and smaller amount of alkanes (boiling range 250-680 ^{o}C, water solubility ca. 1.4-5.8 mg/l).

1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties. For details and references, see European Commission (2000). It is noted, that the study reports were not available to the Rapporteur for evaluation.

REACH ref Annex, §	Property	Value	Comments
VII, 7.1	Physical state at 20 C and 101.3 Kpa	liquid/solid	European Commission, 2000
VII, 7.2	Melting / freezing point	-6 – 36 °C	ASTM, 1991 CONCAWE, 1992
VII, 7.3	Boiling point	250 – 680 °C at 1013 hPa	ASTM, 1991 CONCAWE, 1992
VII, 7.5	Vapour pressure	< 0.1 at 20 °C	CONCAWE, 1992
VII, 7.7	Water solubility	1.4 – 5.8 at 20 °C	CONCAWE, 1992
VII, 7.8	Partition coefficient n-octanol/water (log value)	> 0.5 at 20 °C 4.4-7.2*	Mobil Oil Austria AG Shell Research, 1993
	Dissociation constant	-	

- *value derived experimentally for Dutrex 478FC, CAS No.64742-03-6. pH reported as 6.7; analysis method reversed phase HPLC.

It is noted, that the values presented in Table 1 present those of the whole mixture, whereas the values may not be representative regarding the properties of single constituents and impurities.

2 MANUFACTURE AND USES

Twenty-eight producers/importers have provided data under Regulation 93/793/EEC. The substance is produced/imported in quantities over 1,000,000 tons per year. The notified industrial uses include: basic industry: basic chemicals, fuel industry, polymers industry, rubber manufacturing

industry, asphalt industry and paving/roofing industry. Use categories are: petroleum refining, rubber compounding, fuel/fuel component, intermediates, process regulators, softeners, viscosity adjustors, and vulcanizing agents

3 CLASSIFICATION AND LABELLING

Classification:

T; R45: May cause cancer (Note H)

The substance is presently classified with Carc. cat 2

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

The constituents and impurities of the substance are not expected to be subject to hydrolysis.

4.1.2 Biotic degradation

Industry has provided following results in the IUCLID (European Commission, 2000).

A closed bottle test result conducted according to 84/449/EEC is available (Shell Research, 1993). “Light naphthenic distillate solvent, extract” (CAS 64742-03-6) was used as test substance, test concentration was 3 mg/l, sodium petroleum sulphonate was used as an emulsifier and the inoculum was predominantly domestic sewage. 0 % degradation was observed in 28 days (measured as BOD). It is noted, that the study report was not available to the Rapporteur for evaluation.

Additionally, results from a modified Sturm test according to 84/449/EEC are available from the same study (Shell Research, 1993). Only one test concentration (20 mg/l) was used and the test substance was “Light naphthenic distillate solvent, extract” (CAS 64742-03-6). Sodium petroleum sulphonate was used as an emulsifier and the inoculum was predominantly domestic activated sludge. 0 % degradation was observed by day 28. It is noted, that the study report was not available to the Rapporteur for evaluation.

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

[1] For example, half life from field studies or monitoring data

Reading across from the test results of two available standard ready biodegradability tests carried out with a similar hydrocarbon distillate (CAS 64742-03-6), extracts (petroleum), heavy paraffin distillate solvent can be concluded to be not readily biodegradable. However, it is noted, that the result may not be representative regarding some constituents or impurities, which are present in the substance in a low concentration. The PAH fraction is expected to be persistent or very persistent (see European Commission, 2007).

4.2 Environmental distribution

Data not reviewed for this report.

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

4.3 Bioaccumulation (B)

4.3.1 Screening data

The logKow range of 4.4-7.2 as derived for the similar hydrocarbon distillate with CAS nr. 64742-03-6 indicate, that the constituents of the substance have a high bioaccumulation potential. BCFWIN and DK-QSAR s for alkylbenzenes C20 (benzene tetradecyl) predict a BCF of 4.7. For C20 PAHs BCF-values of 5000-12,000 are predicted. For possible branched alkyl mono- and polyaromatic constituents dibenzyltoluene (CAS 26898-17-9) and tritert-butylbenzene (CAS 1460-02-2), measured BCFs >> 2000 are available.

4.3.2 Measured bioaccumulation data

No experimental data are available for the substance as such. For possible branched alkyl mono- and polyaromatic constituents dibenzyltoluene (CAS 26898-17-9; see PBT summary fact sheet nr. 43) and tritert-butylbenzene (CAS 1460-02-2), measured BCFs >> 2000 are available. For several representatives of the PAH –fraction, experimental BCFs are available for fish and/or with daphnids up to BCF > 5000 (see European Commission, 2007).

4.3.3 Other supporting information[2]

Data not reviewed.

[2]For example, measured concentrations in biota

4.3.4 Summary and discussion of bioaccumulation

The substance meets the B/vB criteria based on screening data. No experimental data on bioaccumulation are available for the mixture. However, several representatives of the PAH-fraction are bioaccumulative based on experimental data.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

It is noted, that the IUCLID (European Commission, 2000) contains acute and chronic ecotoxicity test results which have been obtained using light naphthenic distillate solvent, extract (CAS 64742-03-6) as a test substance. The acute L(E)C50-values using this substance in the invertebrate and algae tests (where solvent was used) are > 0.1 mg/l.

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

A WAF 96h-LL50 of > 1000 mg/l was obtained for *Oncorhynchus mykiss* in a semistatic test according to OECD 203 (BP, 1994). It is noted, that the study report was not available to the Rapporteur for evaluation.

Long-term toxicity

6.1.1.2 Aquatic invertebrates

Acute toxicity

In an OECD 202 –test with Daphnia magna, a WAF 48h-EC50 of > 1000 mg/l was observed (BP, 1994). It is noted, that the study report was not available to the Rapporteur for evaluation.

Long-term toxicity

In 23 day OECD 202 –test with Daphnia magna, light naphthenic distillate solvent, extract (CAS 64742-03-6) was used as test substance dissolved in acetone. NOEC for reproduction of 0.02 mg/l

was observed (Shell, 1993). It is noted, that the study report was not available to the Rapporteur for evaluation.

6.1.1.3 Algae and aquatic plants

A WAF 72h-EC50 of > 1000 mg/l resulted from anOECD 201 –test with *Scenedesmus subspicatus*. It is noted, that the study report was not available to the Rapporteur for evaluation (Safepharm Laboratories, 1994).

6.1.2 Sediment organisms

No data available.

6.1.3 Other aquatic organisms

The available data on micro-organisms were not evaluated for this report.

6.2 Terrestrial compartment

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: Extracts (petroleum) heavy paraffin distillate solvent fulfils the P/vP criteria based on screening data. The substance did not show any degradation in two standard ready biodegradation tests (tested as such).

Bioaccumulation: The substance meets the B/vB criteria based on screening data. Experimental logKow range is 4.4-7.2 based on read across from a similar substance light naphthenic distillate solvent, extract (CAS 64742-03-6). No experimental data on bioaccumulation are available for the mixture. However, several representatives of the PAH-fraction are bioaccumulative based on experimental data.

Toxicity: The substance does not meet the T criterion based on screening data. Acute experimental data with the mixture are available from standard tests with fish, daphnids and algae using WAF. No effects were observed at the highest loading rates. For the similar substance light naphthenic distillate solvent, extract (CAS 64742-03-6) a NOEC of 0.02 mg/l for invertebrates is available (solvent used) and, furthermore, acute exposure with fish and daphnids provided L(E)C50-values > 0.1 mg/l. It is noted, that the ecotoxicity of single constituents and impurities may be higher and hence no definitive conclusion can be drawn based on the present data. The substance meets the T criterion for human health due to its classification as Cat 2 carcinogen.

Summary: Extracts (petroleum) heavy paraffin distillate solvent fulfils the P/vP criteria based on screening data. It also meets the B/vB criteria based on screening data. The screening criterion for ecotoxicity is not met, but no final conclusion can be drawn, as data are available only on the whole mixture, whereas single consituents may fulfil the T (ecotoxicity) criterion. The T criterion is fulfilled for the human health (Cat 2 carcinogen).

It is concluded, that the substance meets the PBT/vPvB –criteria based on screening data. However, no final conclusion on the PBT/vPvB-status of the substance was drawn in the TC NES Subgroup. Further PBT cathegorisation of the UVCB- substance is dependent on guidance development for substances containing PBT or vPvB constituents. Provisionally, extracts (petroleum) heavy paraffin distillate solvent can be regarded as a substance with PBT/vPvB impurities.

INFORMATION ON USE AND EXPOSURE

Not relevant as the substance is not identified as a PBT.

OTHER INFORMATION

The information and references used in this report were taken from the following source:

European Commission, 2000. IUCLID Dataset, Extracts (petroleum), heavy paraffin distillate solvent, CAS 64742-04-7, 18.2.2000.

Other sources:

European Commission, 2007. European Union Risk Assessment Report, Draft of November, 2007, Coal tar pitch, high temperature, CAS No: 65996-93-2, EINECS No: 266-028-2.