CLH report

Proposal for Harmonised Classification and Labelling

Based on Regulation (EC) No 1272/2008 (CLP Regulation), Annex VI, Part 2

Substance Name: **BRANCHED HEXATRIACONTANE**

Synonym: ALKANE 4 or 1-DODECENE TRIMER, HYDROGENATED

EC Number: 417-070-7

CAS Number: 151006-62-1

Index Number: 601-064-00-8

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Part A.

1 PROPOSAL FOR HARMONISED CLASSIFICATION AND LABELLING

1.1 Substance

Table 1: Substance identity

Substance name:	Branched hexatriacontane
EC number:	417-070-7
CAS number:	151006-62-1
Annex VI Index number:	601-064-00-8
Degree of purity:	100% as UVCB

1.2 Harmonised classification and labelling proposal

Table 2: The current Annex VI entry and the proposed harmonised classification

	CLP Regulation
Current entry in Annex VI, CLP Regulation	Aquatic Chronic 4; H413 - May cause long lasting harmful effects to aquatic life
Current proposal for consideration by RAC	Not classified
Resulting harmonised classification (future entry in Annex VI, CLP Regulation)	Not classified

1.3 Proposed harmonised classification and labelling based on CLP Regulation

Only the environmental classification has been considered in this proposal.

Table 3: Proposed classification

CLP Annex I ref	Hazard class	Proposed classification	Proposed SCLs and/or M-factors	Current classification[1)]	Reason for no classification [2)]
2.1.	Explosives	-	-	-	Not considered in this dossier
2.2.	Flammable gases	-	-	-	Not considered in this dossier
2.3.	Flammable aerosols	-	-	-	Not considered in this dossier
2.4.	Oxidising gases	-	-	-	Not considered in this dossier
2.5.	Gases under pressure	-	-	-	Not considered in this dossier
2.6.	Flammable liquids	-	-	-	Not considered in this dossier
2.7.	Flammable solids	-	-	-	Not considered in this dossier
2.8.	Self-reactive substances and mixtures	-	-	-	Not considered in this dossier
2.9.	Pyrophoric liquids	-	-	-	Not considered in this dossier
2.10.	Pyrophoric solids	-	-	-	Not considered in this dossier
2.11.	Self-heating substances and mixtures	-	-	-	Not considered in this dossier
2.12.	Substances and mixtures which in contact with water emit flammable gases	-	-	-	Not considered in this dossier
2.13.	Oxidising liquids	-	-	-	Not considered in this dossier
2.14.	Oxidising solids	-	-	-	Not considered in this dossier
2.15.	Organic peroxides	-	-	-	Not considered in this dossier
2.16.	Substance and mixtures corrosive to metals	-	-	-	Not considered in this dossier
3.1.	Acute toxicity - oral	-	-	-	Not considered in this dossier
	Acute toxicity - dermal	-	-	-	Not considered in this dossier
	Acute toxicity - inhalation	-	-	-	Not considered in this dossier
3.2.	Skin corrosion / irritation	-	-	-	Not considered in this dossier
3.3.	Serious eye damage / eye irritation	-	-	-	Not considered in this dossier
3.4.	Respiratory sensitisation	-	-	-	Not considered in this dossier
3.4.	Skin sensitisation	-	-	-	Not considered in this dossier
3.5.	Germ cell mutagenicity	-	-	-	Not considered in this dossier
3.6.	Carcinogenicity	-	-	-	Not considered in this dossier
3.7.	Reproductive toxicity	-	-	-	Not considered in this dossier
3.8.	Specific target organ toxicity –single exposure	-	-	-	Not considered in this dossier
3.9.	Specific target organ toxicity – repeated exposure	-	-	-	Not considered in this dossier
3.10.	Aspiration hazard	-	-	-	Not considered in this dossier
4.1.	Hazardous to the aquatic environment	Not classified	-	Aquatic Chronic 4 (H413: May cause long lasting harmful effects to aquatic life)	Conclusive but not sufficient for classification
5.1.	Hazardous to the ozone layer	-	-	-	Not considered in this dossier

[1)] Including specific concentration limits (SCLs) and M-factors
[2)] Data lacking, inconclusive, or conclusive but not sufficient for classification

Labelling:

Signal word: None

Hazard statements: None

Precautionary statements: None

Proposed notes assigned to an entry: None

1.4 History of the previous classification and labelling

Branched hexatriacontane was notified in the UK under the Notification of New Substances Regulations (95-06-0721 and 96-06-0808). Branched hexatriacontane was included in Annex I to DSD. At that time, the classification was based on the lack of chronic data along with uncertainties regarding rapid degradation and high bioaccumulation potential. As a poorly water soluble substance, which does not exert acute toxicity at the limit of solubility, branched hexatriacontane was assigned a precautionary classification of R53 'May cause long term adverse effects in the aquatic environment' under DSD. This was translated to Chronic Category 4; H413 – May cause long lasting harmful effects to aquatic life, under the CLP Regulation.

The substance is registered under REACH and the information in this proposal is consistent with the information in the registration dossier.

1.5 Short summary of the scientific justification for the CLH proposal

This report proposes to remove the current harmonised environmental classification for branched hexatriacontane. The substance is not currently classified for physical-chemical properties or human health hazards and these are not considered in this report.

Chronic category 4 applies where classification under the criteria for chronic categories 1-3 do not apply but there are grounds for concern, for example poorly soluble substances for which the L(E)C50 are above the water solubility and which are not rapidly degradable and have a BCF of greater than or equal to 500 (log Kow ≥4). However, other scientific evidence can be used to show classification to be unnecessary, for example chronic toxicity NOEC above the water solubility or other evidence of rapid degradation.

As the substance is not rapidly degradable, the environmental declassification of branched hexatriacontane relies on showing that the substance either is not chronically toxic or has a BCF below the classifiable threshold.

There is no study available directly on the bioaccumulation of branched hexatriacontane. However, the larger olefins are expected to have a lower potential to be bioavailable to aquatic organisms due to their low water solubilities (US EPA 2005). This argument is supported by the results of the report by Girling (2007), which shows that for carbon numbers greater than 15, the BCF is likely to be below 10. In addition, for branched hexatriacontane, a QSAR model gives an estimated BCF of 3.162 L/kg on the basis of the QSAR estimated log Kow (17.87). Further, the REACH guidance notes that, for PBT assessments, a calculated log Kow of 10 or above is taken as an indicator of reduced bioconcentration (REACH Chapter R.7c, ECHA 2014). Thus, it can be concluded that branched hexatriacontane would have a low potential for bioaccumulation.

For chronic aquatic toxicity, experimental data are available for branched hexatriacontane for toxicity to algae (96 hour NOEC). As there are no other chronic data available, data on the long-term toxicity to aquatic invertebrates have been read across from structurally similar substances '1-decene, dimmers, hydrogenated' and '1-decene, homopolymer, hydrogenated' which cover the carbon number range of the branched hexatriacontane. The available data demonstrate that chronic effects are not observed at the limit of solubility (Handley et al 1995, Putt 2003a, b). In addition, QSAR estimates for chronic toxicity to fish, invertebrates and algae are also available for poly alpha olefins of C14 and above which support the argument that chronic toxicity NOEC are above the water solubility. Therefore, due to its predicted lack of effects even after prolonged exposure, environmental classification is not required for branched hexatriacontane.

1.6 Current harmonised classification and labelling

1.6.1 CURRENT CLASSIFICATION AND LABELLING IN ANNEX VI, TABLE 3.1 IN THE CLP REGULATION

Aquatic Chronic 4; H413 - May cause long lasting harmful effects to aquatic life

P273: Avoid release to the environment.

P501: Dispose of contents/container to...

1.7 Current self-classification and labelling

1.7.1 CURRENT SELF-CLASSIFICATION AND LABELLING BASED ON THE CLP REGULATION CRITERIA

The substance is currently classified and labelled in accordance with the harmonised entry. However, this proposal aims to remove the existing classification.

2 JUSTIFICATION THAT ACTION IS NEEDED AT COMMUNITY LEVEL

Branched hexatriacontane has an existing entry on Annex VI of CLP. The agreed classification was considered appropriate at that time due to the lack of chronic data, along with uncertain rapid degradation and bioaccumulation potential. As a poorly water soluble substance, which does not exert acute toxicity at the limit of solubility, branched hexatriacontane was therefore assigned a precautionary classification of R53 'May cause long term adverse effects in the aquatic environment' under the DSD and Chronic Category 4; H13 – May cause long lasting harmful effects in the aquatic environment under CLP.

It is considered that this precautionary classification is not required for branched hexatriacontane. Experimental data indicate that the 96 hour NOEC for algae, based on the nominal loading rate of the water accommodated fraction, is above the water solubility (Handley et al 1995). Data read across from structurally similar substances '1-decene, dimmers, hydrogenated' and '1-decene, homopolymer, hydrogenated' are also available which demonstrate that chronic toxicity to aquatic invertebrates is not observed at the limit of solubility (Putt 2003a and 2003b). These data are further supported by QSAR predictions for poly alpha olefins of C14 and above indicating no chronic toxicity to fish, invertebrates or algae at the limit of water solubility.

As such, this dossier proposes to revise the current harmonised classification of Aquatic Chronic 4; H413 – May cause long lasting harmful effects in the aquatic environment to no classification for environmental hazards.

This proposal has been prepared by Chevron Phillips Chemicals International N.V. (CPC) and submitted by the UK CA in accordance with Article 37(6) of CLP.

Part B.

SCIENTIFIC EVALUATION OF THE DATA

1 IDENTITY OF THE SUBSTANCE

1.1 Name and other identifiers of the substance

Table 4: Substance identity

EC number:	417-070-7
EC name:	Branched hexatriacontane
CAS number (EC inventory):	151006-62-1
CAS number:	151006-62-1
CAS name:	1-Dodecene trimer, hydrogenated
IUPAC name:	Branched hexatriacontane
Synonym:	'Alkane 4'
CLP Annex VI Index number:	601-064-00-8
Molecular formula:	Hill formula: $C_{36}H_{74}$ CAS formula: $C_{36}H_{74}$
Molecular weight range:	506.0

Structural formula: UVCB substance.

The substance is comprised of a mixture of branched C36 alkane isomers, derived from 1-dodecene feedstock. It typically contains >92% hexatriacontane (C36 alkyl), <0.6% tetracosane (C24 alkyl) and <8% octatetracontane (C48 alkyl), but also contains thousands of more complex branched isomers. See below for further information on the known composition.

1.2 Composition of the substance

Table 5: Constituents (non-confidential information)

Constituent	Typical concentration	Concentration range	Remarks
Branched hexatriacontane EC no.: 417-070-7	ca. 95.0 % (w/w)	>= 92.0 — <= 98.0 % (w/w)	C36-alkyl
Tetracosane EC no.: 211-474-5	ca. 0.3 % (w/w)	0.0 — 1.0 % (w/w)	C24-alkyl
Octatetracontane	ca. 4.0 % (w/w)	>= 2.0 — <= 8.0 % (w/w)	C48-alkyl

There are no impurities or additives present in the substance (non-confidential information).

1.2.1 COMPOSITION OF TEST MATERIAL

Branched hexatriacontane is a UVCB substance comprising a mixture of branched C36 alkanes derived from 1-dodecene feedstock. It typically contains >92% hexatriacontane, <0.6% tetracosane, <8% octatetracontane but also contains thousands of more complex branched isomers.

Branched hexatriacontane belongs to the Poly Alpha Olefin (PAO) category. The Poly Alpha Olefins category covers products that are made from the polymerization/oligomerization of alpha olefins (e.g. 1-decene, 1-dodecene and 1-tetradecene). The carbon number range typically ranges from C20 to C60 but may go as high as 84. Products in this category may be hydrogenated to remove remaining double bonds.

The ecotoxicity of Poly Alpha Olefins with the same carbon number is expected to be similar, irrespective of the positioning of any double bonds. The reason for this is that they are neutral organic hydrocarbons which act via non-polar narcosis. Toxicity is due to the uptake of the chemical (proportional to log Kow) and then disruption of the function of biological membranes (US EPA 2005).

Ecotoxicity data for branched hexatriacontane have been read across from the HOPA (Higher Olefins and Poly Alpha Olefins) REACH Consortium's Poly Alpha Olefin category members as the substances are all of the same hydrocarbon class. The category members differ from one-another only in carbon chain length. Although branched hexatriacontane was not registered as part of this category, it would clearly fall within the category domain.

The physico-chemical and environmental fate properties of the category members are similar or change in a predictable fashion. For example, the water solubility is expected to decrease as the carbon number increases and the low water solubility of these hydrocarbon products is expected to limit the bioavailability to aquatic organisms thus their aquatic toxicity (US EPA 2005). It can therefore be assumed that poly alpha olefin products within the described carbon number range will behave in a similar manner and that use of read-across is valid. Branched hexatriacontane has a typical carbon number of C36 and acute and chronic ecotoxicity data are presented for poly alpha olefins with a range of carbon numbers covering C36 (see Annex).

1.2.2 PHYSICO-CHEMICAL PROPERTIES

Table 6: Summary of physico-chemical properties

Property	Value	Reference	Comment
State of the substance	Clear liquid	703/029 (Safepharm Laboratories Limited, 1995)	General observations
Melting/freezing point	<-20°C	703/029 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A1
Boiling point	>165-<317°C	703/029 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A2
Relative density	0.818 at 20°C	703/029 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A3
Vapour pressure	2.5x10-7 Pa at 25°C	703/030 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A4
Surface tension	This test was not necessary as the water solubility of the substance is less than 1 mg/L.		
Water solubility	<0.482 mg/L at 20°C	703/029 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A.6 (Flask shaking method)
	<1 E-6 mg/L	#LT 00-001 (Seary, 2000)	Measured - No guideline followed (analytical method)
	<0.1 mg/L at 20°C	Walker and Mullee (2006)	Measured - OECD 105 (flask method), read across from 1-decene, homopolymer, hydrogenated (C30-60)
Partition coefficient n-octanol/water	>3.87 at 20°C	703/029 (Safepharm Laboratories Limited, 1995)	Measured - OECD 107 (Shake Flask Method) / EU Method A.8
	>7.64, extrapolated to > 8	#LT 00-001 (Seary, 2000)	Measured - No guideline followed (HPLC method)
	>6.5 at 20°C	Walker and Mullee (2006)	Measured - OECD 117 (HPLC Method), read across from 1-decene, homopolymer, hydrogenated (C30-60)
	17.87	KOWWIN v1.68 as part of EPISuite v4.1, US EPA 2012	QSAR model – MCI method
Flash point	>300°C	703/031 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A.9 (closed cup)
Flammability	The substance does not contain groups that are indicative of potential reactivity with water or pyrophoric properties. Further, experience with handling and use supports this.		
Explosive properties	A consideration of the structure confirms that the substance does not contain any groups indicative of explosive properties. The oxygen balance is -345		
Self-ignition temperature	362°C	703/031 (Safepharm Laboratories Limited, 1995)	Measured - EU Method A.15
Oxidising properties	A consideration of the structure confirms that the substance does not contain any groups indicative of oxidising properties.		
Granulometry	Substance is a liquid		
Stability in organic solvents	The stability of the substance is not considered to be critical. Based on the structure of the substance it is not expected to hydrolyse, decompose or undergo any redox reactions with common organic solvents.		
Dissociation constant	The substance does not contain any functional groups that dissociate.		
Viscosity (at 40°C)	22-24 cSt	PAO handbook (Chevron Phillips Chemical, 2002)	Calculated based on carbon number (ASTM D2270) from measured value (test method: ASTM D445) on a substance containing 91.9% branched hexatriacontane.

The data on physical properties were obtained from a number of proprietary studies which followed standard guidelines. The use of Klimisch codes (Klimisch et al., 1997) was applied and a reliability code of 1 or 2 was assigned to the key studies. The available data indicate that branched hexatriacontane would have very low water solubility and a very high partition coefficient. As there are no viscosity data on branched hexatriacontane, data have been read across from poly alpha olefins which bracket the carbon chain length range of the substance.

Partition coefficient

The Safepharm Laboratories study has been used as the key partition coefficient study because it follows accepted guidelines (Method A.8 of Commission Directive 92/69/EEC) and has been evaluated as reliability 1 according to the Klimisch codes. The result is supported by the study #LT 00-001, which has been evaluated as reliability 2 according to the Klimisch codes because it was conducted in accordance with generally accepted scientific principles but possibly has incomplete reporting or methodological deficiencies, though these are not considered to affect the quality of the relevant results. The endpoint is further supported by the results from Walker and Mullee (2006) which have been read across from 1-decene, homopolymer, hydrogenated (CAS number 68037-01-4), a member of the polyalpha olefins group with a carbon number range of 30 to 60.

Due to the limitations in the test methods, the partition coefficient tests have provided unbounded results. Therefore, a QSAR model using the Molecular Connectivity Index method has been included as well, which gives an estimated log Kow value of 17.87 (KOWWIN v1.68 as part of EPISuite v4.1, US EPA 2012). Although there is no official domain for the model, branched hexatriacontane (506 g/mol) falls within the molecular weight range of the training set (18.02 – 719.92 g/mol) and the validation dataset (27.03 – 991.15 g/mol).

The experimental partition coefficient results provided unbounded values (>3.87, >6.5 and >7.6) and the QSAR result is very high (17.87). Therefore, assessing all study data available, the log partition coefficient for branched hexatriacontane can more accurately be extrapolated to be >8. The log partition coefficient has been concluded to be >8 and this value has been used within the Chemical Safety Report as it represents the substance more accurately, reflecting all the available data.

The QSAR models are based on, and validated by, using experimental data. Therefore, the boundaries of the datasets are determined by the capabilities of the testing methodologies. As tests cannot be conducted at high partition coefficients, the QSAR models cannot be validated at these values. The same restraints would therefore be placed on QSAR models that are placed on experimental data, with results being reported as unbounded. The conclusions presented for the partition coefficient endpoint are of unbounded values and the modelled results are included as supporting evidence.

The adsorption/desorption (Koc) and bioaccumulation (BCF) results were calculated based on the QSAR estimated log Kow results (log Kow 17.87) and included as supporting evidence, though the conclusion for these endpoints are based on unbounded results or other available data. The aquatic toxicity models provide the same results using the QSAR estimated log Kow (17.87) or the log Kow based on measured data (>8), therefore the aquatic toxicity models were run using a log Kow value of 8. This is consistent with the approach used in the REACH dossiers for poly alpha olefins when the PETROTOX and ECOSAR were run for these substances.

Water solubility

The Safepharm Laboratories study has been used as the key water solubility study because it follows accepted guidelines (Method A.6 of Commission Directive 92/69/EEC) and has been evaluated as reliability 1 according to the Klimisch scoring system. The result is supported by the study #ILT 00-001, which has been evaluated as reliability 2 according to the Klimisch codes because it was conducted in accordance with generally accepted scientific principles but possibly has incomplete reporting or methodological deficiencies, though these are not considered to affect the quality of the relevant results. The endpoint is further supported by the results from Walker and Mullee (2006) which have been read across from 1-decene, homopolymer, hydrogenated (CAS number 68037-01-4), a member of the polyalpha olefins group with a carbon number range of 30 to 60.

The results indicate that branched hexatriacontane has very low solubility in water, with results ranging from <1 $x10^{-6}$ to <0.482 mg/L and therefore, based the most reliable study on the substance itself, the water solubility result has been concluded to be less than 0.482 mg/L (<4.82 $x10^{-4}$ g/L) at 20°C.

2 MANUFACTURE AND USES

2.1 Manufacture

The substance is manufactured outside of the EU.

2.2 Identified uses

The substance is used in synthetic automotive and industrial lubricants within the EU.

3 CLASSIFICATION FOR PHYSICO-CHEMICAL PROPERTIES

Not considered in this dossier.

4 HUMAN HEALTH HAZARD ASSESSMENT

Not considered in this dossier.

5 ENVIRONMENTAL HAZARD ASSESSMENT

5.1 Degradation

5.1.1 STABILITY

No information is available on the stability of branched hexatriacontane. No data are available on phototransformation and branched hexatriacontane is not expected to hydrolyse based on a lack of hydrolysable functional groups.

5.1.2 BIODEGRADATION

5.1.2.1 Biodegradation estimation

5.1.2.2 Screening tests

Table 7: Summary of ready biodegradability data

Method	Result	Comment
Ready biodegradability (OECD 301B CO_2 evolution test)	Not readily biodegradable (19% biodegradation after 28 days)	Mead (2005) – GLP, Klimisch 1. See discussion for further details.
Ready biodegradability (OECD 301B CO_2 evolution test)	Not readily biodegradable (6% biodegradation after 28 days)	Handley and Mead (1995) – GLP, Klimisch 1. See discussion for further details.

5.1.3 SUMMARY AND DISCUSSION OF DEGRADATION

Biodegradation screening studies are available for branched hexatriacontane following OECD Guideline 301B (CO_2 evolution test) (Mead 2005, Handley and Mead 1995). Due to the low solubility of the substance, both tests were prepared using granular silica gel to disperse the substance in the test media. The substance is considered not readily biodegradable, reaching only 19% and 6 % degradation after 28 days at test item concentrations of 11.7 mg/L and 5 mg/L, respectively. The toxicity control in both studies showed the substance not to be inhibitory to micro-organisms.

Mead 2005

The test material, at a concentration of 10 mg C/L, was exposed to activated sewage sludge micro-organisms with culture medium in sealed culture vessels in the dark at 20°C for 28 days. The degradation of the test material was assessed by the determination of CO_2 produced. Control solutions with inoculum and the standard material, sodium benzoate, together with a toxicity control were used for validation purposes.

Data supplied by the Sponsor indicated that the test material was insoluble in water and therefore, preliminary solubility/dispersion work was conducted. Branched hexatriacontane dispersed in purified water with the aid of ultrasonication for 30 minutes formed a slightly cloudy dispersion with an oil slick of test material on the surface. Branched hexatriacontane dispersed in purified water with the aid of high shear mixing at 7500 rpm for 30 minutes formed a slightly cloudy dispersion with a few very small oily globules of test material floating on the surface. Branched hexatriacontane adsorbed onto silica gel (100 mg) and dispersed in purified water with the aid of high shear mixing at 7500 rpm for 30 minutes formed a cloudy white homogenous dispersion. Branched hexatriacontane dispensed onto filter paper and added to purified water formed a colourless water column with oily globules of test material floating on the surface. Branched hexatriacontane dispensed onto a pre-cleaned glass slide and added to purified water formed a clear colourless water column with large oily globules of test material floating on the surface.

On the basis of the preliminary solubility work and following the recommendations of the International Standards Organisation (ISO 1996) and in the published literature (Handley et al,

2002), branched hexatriacontane was prepared by adsorption onto granular silica gel prior to dispersion in the culture medium with the aid of high shear mixing (7500 rpm, 5 minutes) The test material/silica gel/culture medium dispersion was then dispersed in inoculated culture medium and the volume adjusted to give a final concentration of 11.7 mg/L, equivalent to 10 mg carbon/L. Sealed test vessels were prepared in duplicate, alongside blank controls (inoculum with silica gel), inoculum controls (sodium benzoate, 10 mg C/L, with silica gel) and toxicity controls (sodium benzoate and branched hexatriacontane, 20 mg C/L). Dissolved organic carbon (DOC) analysis was conducted on samples from the test and toxicity control vessels on Day 0 and from the control and reference item on Days 0 and 28. DOC analysis of the test material dispersions after dosing was not possible due to the insoluble nature of the test material in water.

The difference between the values for CO2 production at the end of the test for the replicate vessels was <20% and hence satisfied the validation criterion given in the OECD Test Guidelines. Inorganic carbon analysis of the samples from the second absorber vessels on Day 29 confirmed that no significant carry-over of CO_2 in the second absorber vessels occurred. The toxicity control attained 62% degradation after 28 days thereby confirming that the test material was not toxic to the sewage treatment micro-organisms used in the study. Sodium benzoate attained 94% degradation after 28 days thereby confirming the suitability of the inoculum and test conditions. The test material attained 19% degradation after 28 days and therefore cannot be considered to be readily biodegradable.

Handley and Mead 1995

The test material was exposed to sewage sludge micro-organisms at a concentration of 5 mg C/L with culture medium in sealed culture vessels in the dark at 21°C for 28 days. The degradation of the test material was assessed by the determination of CO_2 produced. Control solutions with inoculum and the standard material, sodium benzoate, together with an abiotic control and toxicity control were used for validation purposes.

Following the recommendations of the Test Guidelines, in the definitive test, the test material concentration was reduced to 5 mg C/L to overcome any possible inhibitory effects of branched hexatriacontane of the activated sewage sludge micro-organisms. It was not possible to test at concentrations below 5 mg C/L as below this concentration it is not possible to distinguish between background CO_2 evolution from the inoculum and CO_2 evolution due to biodegradation when using inorganic carbon analysis.

Following the recommendations of the International Standards Organisation (ISO 1995) and the published literature (Handley et al, 2002), the test material was adsorbed onto granular silica gel prior to dispersion in the test medium to aid dispersion of the test material in the test medium and to increase the surface area of the test material exposed to the test organisms. Observations made throughout the test period showed the contents of the test material vessels were cloudy light brown dispersions with no undissolved test material visible.

Inorganic carbon values for the test material, standard material, toxicity control and control vessels at each analysis occasion were recorded to determine percentage biodegradation and Dissolved Organic Carbon analyses were performed on Days 0 and 28. The total CO_2 evolution in the control vessels on Day 28 was 31.66 mg/L and the IC content of the test material suspension in the mineral medium was below 5% of the TC content. Therefore, the validation criterion given in the OECD Test Guidelines were satisfied. The results of the IC analysis of both absorber vessels on day 29 confirmed that no significant amounts of CO_2 were present in solution in the culture vessels as inorganic carbonate and that there was no significant carry-over of CO_2 into the second absorber.

Sodium benzoate attained 82% degradation after 14 days and 102% degradation after 28 days based on DOC thereby confirming the suitability of the inoculum and test conditions. Branched hexatriacontane attained 6% degradation after 28 days and, therefore, cannot be considered as readily biodegradable.

Read across from poly alpha olefins

In addition, biodegradation screening studies are available for a number of substances in the poly alpha olefin (PAO) category and all have found the test substance not to be readily biodegradable. There is no clear trend in the biodegradability results with increasing carbon number. Based on read across, all of the substances in this category are considered not to be readily biodegradable. However, a wide range in results has been reported, ranging from 0 - 88% over 28 days. Two of the studies (Douglas and Sewell, 1989 and McGoldrick and Mehta, 1992) only narrowly miss the criteria to be considered readily biodegradable indicating that, although not readily biodegradable, these substances can be expected to be inherently biodegradable.

Conclusion

On the basis of the available data, branched hexatriacontane is considered not readily biodegradable and therefore no further discussion of the persistence of the substance is included in the proposal to change the environmental classification.

5.2 Environmental distribution

5.2.1 ADSORPTION/DESORPTION

Table 8: Summary of adsorption/desorption data

Method	Result	Comment
QSAR (EPISuite KOCWIN v2.00)	Koc: 3,222,800,000,000,000 Log Koc: 15.509	Using calculated log Kow of 17.87 for branched hexatriacontane. See discussion for further details.
QSAR (EPISuite KOCWIN v2.00)	Koc: 7,041,000,000 Log Koc: 9.8476	Using calculated MCI method for branched hexatriacontane. See discussion for further details.

Branched hexatriacontane is a member of the Poly Alpha Olefin (PAO) category, members of which expected to adsorb strongly to soils and sediment based on a log Kow >3. A measured Koc is not available for any member of this category but soil sorption of non-ionic substances can be estimated by QSAR models.

QSAR models have been developed that calculate the Koc of non-polar hydrocarbons on the basis of their log Kow, following the clear trend of increasing log Koc with increasing log Kow. For branched hexatriacontane, the QSAR model (KOCWIN program v2.00 within EPISuite v4.11 US EPA 2012) was run on the QSAR estimated log Kow (17.87). The QSAR model gives an estimated Koc of 3.2228 $x10^{+15}$ L/kg, which is equivalent to a log Koc of 15.5090. Although there is no official domain for the model, branched hexatriacontane (506 g/mol) falls within the molecular weight range of the training set (32.04 – 665.02 g/mol) and just outside the validation dataset (73.14 – 504.12 g/mol). The estimated log Kow (17.87) and log Koc (15.5) values for branched

hexatriacontane are outside of the range of those in the model datasets (-5.98 to 9.1 and -2.51 to 7.9 respectively).

In addition, as the experimental log Kow values for the substance are unbounded (concluded to be >8 based on >3.87 (Safepharm 1995), >6.5 (Walker and Mullee 2006) and >7.64 (Seary 2000)), the QSAR model using the Molecular Connectivity Index method has also been used for branched hexatriacontane. The QSAR model (KOCWIN program v2.00 within EPISuite v4.11 US EPA 2012) gives an estimated Koc of 7.041 $x10^{+9}$ L/kg, which is equivalent to a log Koc of 9.85, using the MCI method. Although there is no official domain for the model, branched hexatriacontane (506 g/mol) falls within the molecular weight range of the training set (32.04 – 665.02 g/mol) and just outside the validation dataset (73.14 – 504.12 g/mol). The estimated log Koc value for branched hexatriacontane is outside of the range of those in the model dataset (0 to 6.36).

The QSAR results based on the estimated log Kow for branched hexatriacontane of 17.87 give a log Koc of 15.5 and the QSAR results based on the MCI method give a log Koc for branched hexatriacontane of 9.85. Although branched hexatriacontane falls within the molecular weight range of the training set and only just outside the range of the validation set, the predicted log Kow and log Koc values are outside of the model dataset. It is therefore concluded that branched hexatriacontane has a log Koc of >6.4 (the highest log Koc in the dataset for the MCI model).

5.2.2 VOLATILISATION

No data are available.

5.2.3 DISTRIBUTION MODELLING

No data are available

5.3 Aquatic Bioaccumulation

5.3.1 AQUATIC BIOACCUMULATION

5.3.1.1 Bioaccumulation estimation

Table 9: Summary of bioaccumulation data

Method	Result	Comment
Expert report using QSAR regression-based model	BCF: <10	Girling (2007). See discussion for further details.
QSAR model (BCFBAF v3.01 within EPISuite v4.11 US EPA 2012	BCF: 3.162 L/kg Log BCF: 0.5	Using calculated log Kow of 17.87 for branched hexatriacontane. See discussion for further details.

In accordance with Column 2 of REACH Annex IX, the bioaccumulation study does not need to be conducted if the substance has a low potential to cross biological membranes.

5.3.1.2 Measured bioaccumulation data

No data are available.

5.3.2 SUMMARY AND DISCUSSION OF AQUATIC BIOACCUMULATION

There are no data available directly on the bioaccumulation of branched hexatriacontane. However, the larger olefins are expected to have a lower potential to be bioavailable to aquatic organisms due to their low water solubilities (US EPA 2005). This argument is supported by the results of the report by Girling (2007), which investigated methods of predicting the bioaccumulation of linear, branched and cyclic alkanes for development of QSARs.

In the Girling (2007) report, 10 substances ranging from C6 to C15 were used to develop the QSAR model, which was validated by comparison of predictions for a linear C15 substance to measured data. The relationship between carbon number and BCF described by the model shows that for carbon numbers greater than 15, the BCF is likely to be below 10. Branched hexatriacontane comprises of components with carbon numbers of C24 and above, and these are predominantly C36 and above, and therefore is predicted to have a BCF of less than 10.

For branched hexatriacontane, a QSAR model (BCFBAF v3.01 within EPISuite v4.11 US EPA 2012) was run on the basis of the QSAR estimated log Kow (17.87). The QSAR model gives an estimated BCF of 3.162 L/kg, which is equivalent to a log BCF of 0.5. Although there is no official domain for the model, branched hexatriacontane (506 g/mol, BCF 0.5) falls within the molecular weight range of the data set (68.08 – 991.8 g/mol) and the log BCF range of the dataset (-0.21 – 4.5). The estimated log Kow value for branched hexatriacontane (17.87) is outside of the range of those in the model datasets (-6.5 – 11.26). However, even using the highest log Kow in the BCF model dataset (11.26), branched hexatriacontane would only have a log BCF of 1.44 (BCF of 27.5 L/kg).

Also, a QSAR estimate gives a log Kow value of 17.87 (KOWWIN v1.68 as part of EPISuite v4.1, US EPA 2012) and the REACH guidance notes that, for PBT assessments, a calculated log Kow of 10 or above is taken as an indicator of reduced bioconcentration (REACH Chapter R.7c, ECHA 2014). As the experimental octanol-water partition coefficient data for branched hexatriacontane are unbounded, these cannot be used for direct comparison to this criterion. However, the QSAR estimated log Kow of 17.87 is significantly higher than 10, thus, it can be concluded that branched hexatriacontane would have a low potential for bioaccumulation.

On the basis of the available data, branched hexatriacontane is considered to have a low potential for bioaccumulation, with an estimated BCF of <10.

5.4 Aquatic toxicity

Experimental data on branched hexatriacontane

Aquatic toxicity data are available for branched hexatriacontane for fish, invertebrates and algae. Due to the low water solubility of the substance, all the tests were conducted using Water Accommodated Fractions (WAF) and results are therefore reported as nominal loading rates. No toxicity was observed at any loading rate so the L(E)C50 (nominal loading rate) were determined to be greater than the highest concentration tested. The results are presented in the following table:

Table 10: Summary of ecotoxicity data on branched hexatriacontane

Method	Results	Comment
OECD 203 - *Oncorhynchus mykiss*, freshwater, semi-static, based on mortality	LC50 (96 h): >1000 mg/L (nominal loading rate)	Handley, Sewell and Bartlett (1995) – GLP, Klimisch 1, prepared as Water Accommodated Fraction. See discussion for further details.
OECD 202 – *Daphnia magna*, freshwater, static, based on mobility	EC50 (48 h): >1000 mg/L (nominal loading rate)	Handley, Wetton and Bartlett (1995) – GLP, Klimisch 1, prepared as Water Accommodated Fraction. See discussion for further details.
OECD 201 - *Pseudokirchneriella subcapitata*, freshwater, static, based on growth rate and biomass	EC50 (96 h): >1000 mg/L (nominal loading rate WAF) NOEC (96 h): ≥1000 mg/L (nominal loading rate)	Handley, Mead and Bartlett (1995) – GLP, Klimisch 1, prepared as Water Accommodated Fraction. See discussion for further details.

In view of the difficulties associated with the evaluation of aquatic toxicity for poorly water soluble complex mixtures, the approach recommended by CONCAWE for oil products (Concawe 1993) and subsequently endorsed by several important regulatory authorities in the EC (UK Department of Environment 1993, Dutch Directorate of Chemicals 1992) and elsewhere, is to expose organisms to the "Water Accommodated Fraction" (WAF) of the oil product. Using this approach, aqueous medium is prepared by mixing the product with water for a prolonged period (usually 24 hours), with continuous stirring to ensure equilibration between the product and water phase. At the completion of mixing, the product phase is separated and organisms exposed to the aqueous phase (which will contain dissolved material, along with any part of the product that may be present in emulsified or dispersed form). Exposures are expressed in terms of the original concentration of product in water at the preparation of the WAF (the loading rate), irrespective of the actual concentration of product dissolved in water.

For all three studies, the following methods of analysis were attempted during pre-study method development: Gas chromatography - mass spectrometry (GC-MS), GC-MS using Total Ion Chromatogram (TIC) and subsequently Selected Ion Monitoring (SIM). The results of the analysis showed the concentration of the test material in the WAF to be no higher than background levels of hydrocarbon exhibited in the control samples and analysis of the test and control samples showed that the solubility of many of the components of branched hexatriacontane in aqueous media is lower than the limit of quantification (0.04 mg/L). For analysis during the definitive studies, the total organic carbon was determined in the 1000 mg/L loading rate WAF. Given the background level of carbon in the control vessels and the low level of carbon in the test vessels, it is considered that all the results were around the limit of detection of the analytical method.

The definitive acute toxicity to fish study on *Oncorhynchus mykiss* was conducted as limit test, consisting of a semi-static study with two replicates, which were closed to reduce evaporation, and daily renewal of test solutions at a single concentration (1000 mg/L WAF). The test concentration was determined on the basis of a preliminary range finding study at loading rates of 100 and 1000 mg/L WAF. For analysis during the study, the total organic carbon was determined at 0 hours (fresh preparations), 24 hours (old preparations), 72 hours (fresh preparations) and 96 hours (old preparations).

The definitive acute toxicity to invertebrates study on *Daphnia magna* was conducted as a limit test, consisting of a static study with four test replicates, which were closed to reduce evaporation, and test solutions at a single concentration (1000 mg/L WAF). The test concentration was determined on the basis of a preliminary range finding study at loading rates of 100 and 1000 mg/L WAF. For analysis during the study, the total organic carbon was determined at 0 hours (fresh preparations) and 48 hours (old preparations).

For the purpose of the definitive acute toxicity to fish and invertebrates studies, the test material was prepared as a WAF. Approximately 24 hours prior to the study start an amount of test material was dispensed onto the surface of the appropriate volume of dechlorinated tap water to give a 1000 mg/L loading rate and stirred for 20 hours. The stirring rate (rpm) of the magnetic stirrer and the depth of the vortex (approximately 20-25% of the depth of the mixing vessel for test solutions) were recorded at the start and finish of the stirring period. The mixture was allowed to stand for 4 hours prior to removal of the aqueous phase for testing. During the 4 hour standing phase, the test material was observed at the water surface only and during the test, the WAF was observed to be a clear, colourless solution. The results of preliminary investigations showed that there was no significant increase in the carbon concentrations of the WAF by extending the stirring period from 24 to 48 hours and therefore it was considered justifiable to use the 24 hour stirring period for the study. It was considered unnecessary and unrealistic to test at concentrations in excess of 1000 mg/L WAF.

The definitive algal growth inhibition study, using *Selenastrum capricornutum* (new name: *Pseudokirchneriella subcapitata*), was conducted as a limit test, consisting of a static study with six test replicates, which were closed to reduce evaporation, and test solutions at a single concentration (1000 mg/L WAF). The test concentration was determined on the basis of a preliminary range finding study at a loading rate of 1000 mg/L WAF. For analysis during the study, the total organic carbon was determined at 0 hours (fresh preparations) and 96 hours (old preparations) in separately prepared solutes of WAF diluted 50:50 with culture medium to avoid an increase in the carbon concentration resulting from the algal cells.

For the purpose of the definitive algal growth inhibition study, the test material was prepared as a WAF. Approximately 24 hours prior to the study start an amount of test material was dispensed onto the surface of the appropriate volume of culture medium water to give a 2000 mg/L loading rate and stirred for 20 hours. The stirring rate (rpm) of the magnetic stirrer and the depth of the vortex (approximately 20-25% of the depth of the mixing vessel for test solutions) were recorded at the start and finish of the stirring period. The mixture was allowed to stand for 4 hours prior to removal of the aqueous phase for testing. Appropriate volumes of the WAF were then diluted 50:50 with the algal suspension to give a final test concentration of 1000 mg/L WAF. It was considered unnecessary and unrealistic to test at concentrations in excess of 1000 mg/L WAF.

<u>Experimental data read across from poly alpha olefins</u>

In addition to the data for branched hexatriacontane, data are available for a range of poly alpha olefins for acute toxicity to fish, invertebrates and algae and chronic toxicity to invertebrates and algae (see Annex). Due to the low water solubility of the substances all the tests are conducted

using Water Accommodated Fractions (WAF) or Oil Water Dispersions (OWD) and results are therefore reported as nominal loading rates. No toxicity was observed at any loading rate so the NOEC (nominal loading rate) were determined to be equal to or greater than the highest concentration tested and the L(E)C50 (nominal loading rate) were determined to be greater than the highest concentration tested.

The key read across data have been used to complete the chronic toxicity to aquatic invertebrates endpoint as no data were available for branched hexatriacontane. Putt (2003) is a GLP-compliant semi-static full life-cycle toxicity test with *Daphnia magna* following OECD 211. The results show that following a 21-day exposure, there was no adverse effect observed on survival, growth or reproduction and so the NOELR is 125 mg/L nominal loading rate WAF.

The study was conducted on 1-decene homopolymer hydrogenated (CAS 68037-01-4) and read across to branched hexatriacontane. These substances are both members of the Poly Alpha Olefins category, members of which are all of the same hydrocarbon class. The hydrogenated materials are saturated hydrocarbons with some branching. The primary difference between category members is the carbon number range. The carbon chains typically range from C16 to C60 in length, with or without hydrogenation. The physico-chemical and environmental fate properties are similar across the category or change in a predictable fashion and environmental effects are similar, acting via non-polar narcosis, though it is expected that the low water solubility of the products will limit the potential aquatic toxicity. It can therefore, be assumed that products meeting the applicable domain will behave in a similar manner and that use of read-across is valid.

QSAR models

As the experimental data are only available as WAF or OWD, supporting ECOSAR and PETROTOX QSAR predictions were also determined for acute and chronic toxicity of poly alpha olefins to fish, invertebrates and algae. The QSAR results for long chain poly alpha olefins predict that with increasing carbon number and increasing log Kow values, the aquatic toxicity and the water solubility decrease. The PETROTOX results for poly alpha olefins of C14 and higher and ECOSAR results for poly alpha olefins with log Kow above 8 predict that no acute or chronic toxicity would be observed. Therefore, acute and chronic toxicity would not be expected for branched hexatriacontane as the carbon number (C36) and the log Kow (>8 based on experimental data and 17.87 based on QSAR estimation) exceed these values.

As the same results were determined in PETROTOX and ECOSAR for all poly alpha olefins of C14 and above with log Kow of >8, the concluded log Kow of >8 was used to determine the QSAR estimated aquatic toxicity of branched hexatriacontane. The aquatic toxicity models were not run for branched hexatriacontane using the QSAR estimated log Kow of 17.87 as this would produce the same results as are already presented using the log Kow of >8, determined from the experimental data.

PETROTOX

The PETROTOX QSAR predictions were not conducted for branched hexatriacontane specifically but results are presented instead for poly alpha olefins of C14 and higher. The PETROTOX results for poly alpha olefins of C14, for which PETROTOX predicted a log Kow of 7.86, showed that the acute L(E)C50 (reported as L(E)L50) and chronic NOEC (reported as NOEL) were >1000 mg/L. The same lack of toxicity was observed for all longer chain substances in the poly alpha olefins category (with PETROTOX predicted log Kow >8) and therefore branched hexatriacontane (C36 and log Kow >8) is concluded to have an acute L(E)C50 and chronic NOEC of >1000 mg/L as well. Branched hexatriacontane (C36, 506 g/mol, log Kow >8) falls within the carbon number range (4-

41), the molecular weight range (56.1 – 569.1 g/mol) and the log Kow range (2.0 – 21.4) of the model dataset.

ECOSAR

ECOSAR uses the log Kow of the substance as the major physico-chemical attribute correlating a chemical structure to a toxic effect. For acute toxicity, data indicate that, at log Kow values of greater than 5.0 for fish and invertebrates and 6.4 for algae, the decreased solubility results in "no effects at saturation". For chronic toxicity, log Kow values of greater than 8 indicate that the decreased solubility results in "no effects at saturation". Branched hexatriacontane has a log Kow of >8 and therefore exceeds the boundary for acute (log Kow >6.4) and chronic (log Kow >8) QSAR predictions of "no effects at saturation".

Although there is no official domain for the model, the methodology document for ECOSAR states that "in the development of the ECOSAR equations for neutral organics and classes with excess toxicity, the training sets generally include chemicals with log Kow values in the range of -3 to 8 and molecular weights less than 1000. However, the domain of the model is considered to be larger than the descriptor ranges of the training set of chemicals…. It has been determined through empirical data that for acute toxicity endpoints, chemicals with a log Kow value >5.0 are generally expected to have no effects at saturation. For chronic effects, chemicals with a log Kow value >8.0 are expected no effects at saturation. Although the individual equations may not have been not built using chemicals with log Kow values greater than 5.0 and 8.0 respectively, the model can still make accurate qualitative determination of potential toxicity under environmental conditions for chemicals outside the log Kow descriptor domain… Log Kow cut offs can be class specific where data indicated a departure from this general trend of 5.0 for acute effects, and 8.0 for chronic effects. The log Kow limits for each class will be presented in the output file from ECOSAR." The output file from ECOSAR for branched hexatriacontane included the following statement under class specific log Kow cut-offs "If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)

Maximum LogKow: 6.0 (Earthworm LC50)

Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)"

Therefore, the use of the ECOSAR model to predict toxicity of branched hexatriacontane (log Kow of >8) is considered to be robust and no effects at saturation are expected for short-term and long-term toxicity to fish, aquatic invertebrates and algae.

Conclusion

The available data on the substance itself and read across from the poly alpha olefins, as well as the QSAR estimates, indicate that branched hexatriacontane would show no acute or chronic toxicity at the limit of water solubility (<0.482 mg/L). Please see the tables in section 8 for a summary of the available data.

5.4.1 FISH

5.4.1.1 Short-term toxicity to fish

An acute toxicity to fish study is available for branched hexatriacontane (Handley 1995). The GLP-compliant study on *Oncorhynchus mykiss* followed OECD guideline 203, with the test solutions prepared as Water Accommodated Fractions (WAF) due to the low solubility of test item. The 96-hour LC50 (nominal loading rate) is greater than 1000 mg/L WAF and the NOEC (nominal loading rate) is greater than or equal to 1000 mg/L WAF.

In addition to the data for branched hexatriacontane, eight acute fish toxicity studies are available on poly alpha olefins. There does not appear to be any difference in sensitivity between the two species used in the tests: *Oncorhynchus mykiss* and *Cyprinodon variegatus*. Due to the very low solubility of the test substances, all the tests were conducted using Water Accommodated Fractions (WAF) or Oil Water Dispersions (OWD). WAF is the recommended method to test substances with low water solubility and therefore favoured over the studies using OWD. However, all studies report that no effects were seen at the highest concentrations tested. The 96 hour LC50 (nominal loading rate) is therefore concluded to be >1000 mg/L WAF.

To support the experimental data for these poorly soluble substances, QSAR estimates are also available for poly alpha olefins from the PETROTOX and ECOSAR models. The QSAR results for long chain poly alpha olefins predict that with increasing carbon number and increasing log Kow values, the aquatic toxicity and the water solubility decrease. The PETROTOX results for poly alpha olefins of C14 and higher (log Kow >8) showed that the acute LC50 were >1000 mg/L and therefore branched hexatriacontane (C36 and log Kow >8) is concluded to have an acute LC50 of >1000 mg/L as well. The ECOSAR model showed that poly alpha olefins with a log Kow of >5 show no acute toxicity to fish below the limit of water solubility and therefore branched hexatriacontane (log Kow of >8) is expected show no acute toxicity to fish below the limit of water solubility. The modelled LC50 were predicted to be >1000 mg/L (PETROTOX) and > water solubility (ECOSAR). The 96 hour LC50 (nominal loading rate) for poly alpha olefins and branched hexatriacontane is >1000 mg/L WAF.

5.4.1.2 Long-term toxicity to fish

No experimental ecotoxicity data are available for the long-term toxicity of branched hexatriacontane or poly alpha olefins to fish. As such, QSAR estimates have been included for this endpoint using the PETROTOX and ECOSAR models. The QSAR results for long chain poly alpha olefins predict that with increasing carbon number and increasing log Kow values, the aquatic toxicity and the water solubility decrease. The PETROTOX results for poly alpha olefins of C14 and higher (log Kow >8) showed that the chronic NOEC for fish were >1000 mg/L and therefore branched hexatriacontane (C36 and log Kow >8) is concluded to have a chronic NOEC of >1000 mg/L as well. The ECOSAR model showed that poly alpha olefins with a log Kow of >8 show no chronic toxicity to fish below the limit of water solubility and therefore branched hexatriacontane (log Kow of >8) is expected show no chronic toxicity to fish below the limit of water solubility. The chronic NOEC were predicted to be >1000 mg/L (PETROTOX) and > water solubility (ECOSAR).

5.4.2 AQUATIC INVERTEBRATES

5.4.2.1 Short-term toxicity to aquatic invertebrates

An acute toxicity to invertebrates study is available for branched hexatriacontane (Handley 1995). The GLP-compliant study on *Daphnia magna* followed OECD guideline 202, with the test solutions prepared as Water Accommodated Fractions (WAF) due to the low solubility of test item. The 48-hour EC50 (nominal loading rate) is greater than 1000 mg/L WAF and the NOEC (nominal loading rate) is greater than or equal to 1000 mg/L WAF.

In addition, eight acute invertebrate studies are available on poly alpha olefins. There does not appear to be any difference in sensitivity between the six tests conducted with *Daphnia magna* and the two studies with *Mysidopsis bahia*. Due to the very low solubility of the test substances all the tests were conducted using Water Accommodated Fractions (WAF) with results reported as nominal loading rates. All studies report unbounded EC50 (nominal loading rate), with the 50% effect level above the highest concentration tested. The six OECD style tests used higher test concentrations than the two USEPA style tests. Based on the OECD style tests we can conclude that the EC50 (nominal loading rate) is >1000 mg/L WAF.

To support the experimental data for these poorly soluble substances, QSAR estimates are also available for poly alpha olefins from the PETROTOX and ECOSAR models. The QSAR results for long chain poly alpha olefins predict that with increasing carbon number and increasing log Kow values, the aquatic toxicity and the water solubility decrease. The PETROTOX results for poly alpha olefins of C14 and higher (log Kow >8) showed that the acute LC50 were >1000 mg/L and therefore branched hexatriacontane (C36 and log Kow >8) is concluded to have an acute LC50 of >1000 mg/L as well. The ECOSAR model showed that poly alpha olefins with a log Kow of >5 show no acute toxicity to invertebrates below the limit of water solubility and therefore branched hexatriacontane (log Kow of >8) is expected show no acute toxicity to invertebrates below the limit of water solubility. Modelled LC50 were predicted to be >1000 mg/L (PETROTOX) and > water solubility (ECOSAR).

The 48 hour EC50 (nominal loading rate) for poly alpha olefins and branched hexatriacontane is >1000 mg/L WAF.

5.4.2.2 Long-term toxicity to aquatic invertebrates

No experimental ecotoxicity data are available for the long-term toxicity of branched hexatriacontane to aquatic invertebrates and therefore, data have been read across from the poly alpha olefins.

Putt (2003a and 2003b) tested the chronic toxicity of dec-1-ene dimer hydrogenated and 1-decene homopolymer hydrogenated to *Daphnia magna* in OECD Guideline 211 tests. Due to the low solubility of the test substances, the tests were conducted as semi-static tests with Water Accommodated Fractions (WAF) with results based on nominal loading rates. Both studies were conducted as limit tests with a single test concentration of 125 mg/L WAF. The endpoints measured were mortality, timing of first brood, number of offspring and length and weight of offspring. No effects were observed on any endpoint in either test. The 21 day NOEC (nominal loading rate) is therefore ≥125 mg/L WAF.

The studies were conducted as limit tests, consisting of semi-static studies, each with 10 test replicates of test solutions at a single nominal loading rate (mass of test substance per water volume used in WAF preparation) of 125 mg/L. The protocol for the studies states that loading rates in the

definitive study are based on the results of a preliminary range-finding test; “if the substance showed no toxicity in the range finding test, the definitive test will be conducted at a single concentration of 125 mg/L.” No results were presented in the study reports for range-finding studies.

The test solutions were prepared daily by adding the test substance directly into the test water and stirring for 48 hours. The stirring rate (rpm) of the magnetic stirrer was such that there was no vortex. The mixture was allowed to stand for 1 hour prior to removal of the aqueous phase directly into each test vessel via an outlet port 2 cm from the bottom of the jar. After settling, the WAF were observed to be a clear, colourless solution with no visible undissolved test substance.

No information on the solubility of the substance is included in the study report, though it was noted that due to the low solubility and the lack of appropriate sensitivity in the analytical method, analytical measurement of WAFs was determined not to be feasible. Several attempts using different chromatographic techniques (GPC/ELSD, GPC/UV, GC/FID) and a solid phase extraction (SPE) technique were attempted by injecting prepared standards or sample extracts onto the instruments to evaluate the approximate sensitivity of the methodology.

The substance tested in the study by Putt (2003b) consists of 1-decene trimer, tetramer, pentamer, hexamer, etc. (C30-C60) which covers the carbon chain length of branched hexatriacontane (predominantly C36, with some C48). The majority components of the tested item are 1-decene trimer (C30) and 1-decene tetramer (C40) which bracket the carbon number of branched hexatriacontane (C36). The tested substance is also a UVCB with a similar type and extent of branching. Furthermore, the Putt (2003a) study on 1-decene, dimers, hydrogenated (C20) showed no chronic toxicity at the limit of solubility, which demonstrated the lack of chronic toxicity of substances with lower carbon numbers than the tetracosane (C24) constituent of branched hexatriacontane. Hence by interpolation of the data covering a larger carbon chain range (C20 to C60) than branched hexatriacontane (C24 to C48), the lack of chronic aquatic toxicity from these studies has been read across to branched hexatriacontane.

To support the experimental data for these poorly soluble substances, QSAR estimates are also available for poly alpha olefins from the PETROTOX and ECOSAR models. The QSAR results for long chain poly alpha olefins predict that with increasing carbon number and increasing log Kow values, the aquatic toxicity and the water solubility decrease. The PETROTOX results for poly alpha olefins of C14 and higher (log Kow >8) showed that the chronic NOEC for invertebrates were >1000 mg/L and therefore branched hexatriacontane (C36 and log Kow >8) is concluded to have a chronic NOEC of >1000 mg/L as well. The ECOSAR model showed that poly alpha olefins with a log Kow of >8 show no chronic toxicity to invertebrates below the limit of water solubility and therefore branched hexatriacontane (log Kow of >8) is expected show no chronic toxicity to invertebrates below the limit of water solubility. Modelled chronic NOEC were predicted to be >1000 mg/L (PETROTOX) and > water solubility (ECOSAR).

The 21 day NOEC (nominal loading rate) for poly alpha olefins and branched hexatriacontane is 125 mg/L WAF.

5.4.3 ALGAE AND AQUATIC PLANTS

An algal growth inhibition study is available for branched hexatriacontane (Handley 1995). The GLP-compliant study on *Pseudokirchneriella subcapitata* followed OECD guideline 201, with the test solutions prepared as Water Accommodated Fractions (WAF) due to the low solubility of test item. The 96-hour EC50 (nominal loading rate) is greater than 1000 mg/L WAF and the NOEC (nominal loading rate) is greater than or equal to 1000 mg/L WAF.

Three algal toxicity tests are available for the poly alpha olefins, two of which follow OECD guideline 201 (Mattock 1995e, f) and one which follows EPA OTS 797.1050 (Algal Toxicity, Tiers I and II) (Forbis 1990). The studies were conducted on substances in the HOPA Consortium, covering a range of chain lengths from 'dec-1-ene, dimmers, hydrogenated' (C20) to '1-decene, homopolymer, hydrogenated' (C30-C60). The tests were conducted over 72 -96 hours using *Pseudokirchneriella subcapitata* (reported as *Selenastrum capricornutum*). Due to the very low solubility of the test substances all the tests were conducted using Water Accommodated Fractions (WAF) with results reported as nominal loading rates. All studies report that no effects were seen at the highest concentration tested, with a NOEC (nominal loading rate) of 1000 mg/L WAF. As the NOEC (nominal loading rate) are the highest concentration tested, the EC50 (nominal loading rate) can be concluded as unbounded, with a value of >1000 mg/L WAF.

To support the experimental data for these poorly soluble substances, QSAR estimates are also available for poly alpha olefins from the PETROTOX and ECOSAR models. The QSAR results for long chain poly alpha olefins predict that with increasing carbon number and increasing log Kow values, the aquatic toxicity and the water solubility decrease. The PETROTOX results for poly alpha olefins of C14 and higher (log Kow >8) showed that the acute EC50 and chronic NOEC were >1000 mg/L and therefore branched hexatriacontane (C36 and log Kow >8) is concluded to have an acute EC50 and a chronic NOEC of >1000 mg/L as well. The ECOSAR model showed that poly alpha olefins with a log Kow of >6.5 show no acute toxicity to algae below the limit of water solubility and poly alpha olefins with a log Kow of >8 show no chronic toxicity to algae below the limit of water solubility. Therefore, branched hexatriacontane (log Kow of >8) is expected show no acute or chronic toxicity to algae below the limit of water solubility. Modelled EC50 and NOEC were predicted to be >1000 mg/L (PETROTOX) and > water solubility (ECOSAR).

The 72 hour NOEC (nominal loading rate) for poly alpha olefins and branched hexatriacontane is 1000 mg/L WAF.

5.4.4 OTHER AQUATIC ORGANISMS (INCLUDING SEDIMENT)

Data are available for branched hexatriacontane on the toxicity to aquatic micro-organisms and sediment dwelling organisms. Data are also available on poly alpha olefins on the toxicity to aquatic micro-organisms.

The activated sludge respiration inhibition study on branched hexatriacontane (Mead 2000) is a GLP-compliant study on non-adapted activated sludge of a predominantly domestic sewage which followed OECD guideline 209. Following a preliminary range-finding study, activated sewage sludge was exposed to an aqueous dispersion of the test material at 1000 mg/L for 3 hours. The rate of respiration was determined after 30 minutes and 3 hours contact time and compared to data for the control and reference material, 3,5 -dichlorophenol. The 3 hour EC50 (nominal loading rate) is greater than 1000 mg/L and the NOEC (nominal loading rate) is 1000mg/L.

Data are available on the toxicity to aquatic micro-organisms for four poly alpha olefins, covering a range of chain lengths from 'dec-1-ene, dimmers, hydrogenated' (C20) to '1-dodecene, polymer,

with 1-decene, hydrogenated' (C30-C84) (Handley 1995, Douglas 2003, Lebertz 1997). Four of the five results were taken from the toxicity control results in the ready biodegradability studies, which showed no inhibition of the aquatic micro-organisms at the concentrations tested (2 to 23.5 mg/L test item based on nominal loading rates). The fifth result was taken from an investigation of chronic bacterial toxicity according to DIN 38412 Part 8 (Lebertz 1997). *Pseudomonas putida* were exposed to 0.1, 1 and 10 g/L of the test item based on nominal loading rates for 16 hours and no inhibition was observed at the highest concentration tested. The 16 hour EC50 (nominal loading rate) is greater than 10,000 mg/L and the NOEC (nominal loading rate) is 10,000mg/L.

The sediment toxicity study on branched hexatriacontane (Goodband 2009) is a GLP-compliant study on *Chironomus riparius* which followed OECD guideline 218. Following preliminary range-finding tests, larvae were exposed for 28 days to formulated sediment spiked with 100, 180, 320, 560 and 1000 mg/kg test item (nominal loading rate), after which the numbers of emerged adult midges were recorded. The results showed the 28 day EC50 (nominal loading rate) was 420 mg/kg based on emergence and 750 mg/kg based on development rate and the NOEC (nominal loading rate) was 180 mg/kg.

The available information on other aquatic organisms is not considered relevant to the proposed classification change.

5.5 Comparison with criteria for environmental hazards (sections 5.1 – 5.4)

Poorly water soluble substances which do not exert acute toxicity at their limit of solubility and which are not rapidly degradable and have a BCF of greater than or equal to 500 (log Kow ≥4) may require a precautionary classification of Chronic Category 4.

Branched hexatriacontane is not readily biodegradable but it is expected to have a low potential for bioaccumulation. The larger olefins are expected to have a lower potential to be bioavailable to aquatic organisms due to their low water solubilities (US EPA 2005). This argument is supported by the results of the report by Girling (2007), which shows that for carbon numbers greater than 15, the BCF is likely to be below 10. Branched hexatriacontane comprises of components with carbon numbers of C24 and above, and these are predominantly C36 and above, and therefore is predicted to have BCF of less than 10. Also, for branched hexatriacontane, a QSAR model (BCFBAF v3.01 within EPISuite v4.11 US EPA 2012) gives an estimated BCF of 3.162 L/kg, which is equivalent to a log BCF of 0.5, on the basis of the QSAR estimated log Kow (17.87). In addition, the REACH guidance notes that, for PBT assessments, a calculated log Kow of 10 or above is taken as an indicator of reduced bioconcentration (REACH Chapter R.7c, ECHA 2014). On the basis of the available data, branched hexatriacontane is considered to have a low potential for bioaccumulation, with an estimated BCF of <10, and therefore will not meet the criteria of BCF ≥500 for classification as Chronic Category 4.

In addition, the precautionary Chronic Category 4 classification is concluded not to be required for branched hexatriacontane as available data demonstrate that chronic effects are not observed at the limit of solubility (the water solubility for branched hexatriacontane is concluded to be $<4.82 \times 10^{-4}$ g/L at 20°C).

Acute toxicity to fish and invertebrates studies are available for branched hexatriacontane (Handley 1995), which show, respectively, the 96-hour and 48-hour LC50 values (nominal loading rate) are > 1000 mg/L WAF and the NOEC values (nominal loading rate) are ≥1000 mg/L WAF. No experimental ecotoxicity data are available for the long-term toxicity of branched hexatriacontane to fish or invertebrates. Data for long-term toxicity to aquatic invertebrates have been read across from the poly alpha olefins, dec-1-ene dimer hydrogenated (C20) and 1-decene homopolymer

hydrogenated (C30-60) (Putt 2003a and 2003b), which showed no toxicity at the single test concentration tested and therefore, the 21 day NOEC (nominal loading rate) is ≥125 mg/L WAF. This is supported by QSAR estimates for the long-term toxicity to fish and invertebrates, with modelled chronic NOEC predicted to be >1000 mg/L (PETROTOX) and > water solubility (ECOSAR) for branched hexatriacontane. An algal growth inhibition study is available for branched hexatriacontane (Handley 1995), which shows the 96-hour EC50 (nominal loading rate) is > 1000 mg/L WAF and the NOEC (nominal loading rate) is ≥1000 mg/L WAF.

Table 11: Summary of available ecotoxicity data

	Experimental results	**QSAR**
Short-term fish	96-hour LC50 (nominal loading rate) > 1000 mg/L WAF (Handley 1995)	96-hour LC50 > water solubility (ECOSAR) 96-hour LC50 > 1000 mg/L (PETROTOX)
Short-term invertebrates	48-hour LC50 (nominal loading rate) > 1000 mg/L WAF (Handley 1995)	48-hour LC50 > water solubility (ECOSAR) 48-hour LC50 > 1000 mg/L (PETROTOX)
Short-term algae	96-hour EC50 (nominal loading rate) are > 1000 mg/L WAF (Handley 1995)	96-hour EC50 > water solubility (ECOSAR) 96-hour EC50 > 1000 mg/L (PETROTOX)
Long-term fish	-	NOEC > water solubility (ECOSAR) NOEC > 1000 mg/L (PETROTOX)
Long-term invertebrates	21 day NOEC (nominal loading rate) ≥125 mg/L WAF (read across from dec-1-ene dimer hydrogenated (C20) and 1-decene homopolymer hydrogenated (C30-60)) (Putt 2003 a, b)	NOEC > water solubility (ECOSAR) NOEC > 1000 mg/L (PETROTOX)
Long-term algae	96-hour NOEC (nominal loading rate) ≥1000 mg/L WAF (Handley 1995)	NOEC > water solubility (ECOSAR) NOEC > 1000 mg/L (PETROTOX)

Data on branched hexatriacontane and read across from poly alpha olefins indicate that acute and chronic aquatic toxicity is not observed at loading concentrations far in excess of the water solubility (<4.82 x10^{-4} g/L at 20°C). The findings are further confirmed by both PETROTOX and ECOSAR QSAR models, which predict acute L(E)C50 and chronic NOEC for poly alpha olefins of >1000 mg/L and > water solubility, respectively, for fish, invertebrates and algae. On the basis of the available data, it can be concluded that branched hexatriacontane would not cause acute or chronic toxicity to fish, invertebrates or algae at concentrations up to the limit of solubility.

5.6 Conclusions on classification and labelling for environmental hazards

The chronic ecotoxicity data read across from similar substances and QSAR predictions using two different models indicate that a classification is not warranted. As such, it is proposed that no environmental classification is required.

Chronic category 4 is applied when data do not allow classification of a substance as chronic category 1-3 but there are nevertheless grounds for concern, such as poorly water soluble substances for which no acute toxicity is observed at levels up to the water solubility, and which are not rapidly biodegradable and have a BCF ≥500. However, classification shall not be applied where there is evidence this is unnecessary, such as chronic toxicity NOECs higher than the water solubility or other evidence of rapid degradation.

Branched hexatriacontane is not rapidly biodegradable and there is no other evidence of rapid degradation. Although there is no experimental study for bioaccumulation, branched hexatriacontane is concluded to have a low potential for bioaccumulation, with an estimated BCF of <10. The larger olefins are expected to have a lower potential to be bioavailable to aquatic organisms due to their low water solubilities (US EPA 2005). This argument is supported by the results of the report by Girling (2007), which shows that for carbon numbers greater than 15, the BCF is likely to be below 10 (branched hexatriacontane comprises of components with carbon numbers of C24 and above, and these are predominantly C36 and above). Also, for branched hexatriacontane, a QSAR model gives an estimated BCF of 3.162 L/kg on the basis of the QSAR estimated log Kow (17.87). The REACH guidance notes that, for PBT assessments, a calculated log Kow of 10 or above is taken as an indicator of reduced bioconcentration (REACH Chapter R.7c, ECHA 2014). On the basis of the available data, branched hexatriacontane is considered to have a low potential for bioaccumulation, with an estimated BCF of <10, and therefore will not meet the criteria of BCF ≥500 for classification as Chronic Category 4.

Data on branched hexatriacontane and read across from poly alpha olefins indicate that aquatic toxicity is not observed at loading concentrations in excess of the water solubility (<4.82 $x10^{-4}$ g/L at 20°C). No effects were observed at the highest concentrations tested, with acute (fish, invertebrates and algae) and chronic (invertebrates and algae) NOEC ranging from >125 mg/L to >1000 mg/L. The findings are further confirmed by both PETROTOX and ECOSAR QSAR models, which predict acute L(E)C50 and chronic NOEC values of >1000 mg/L and > water solubility, respectively, for fish, invertebrates and algae. On the basis of the available data, it can be concluded that branched hexatriacontane would not cause acute or chronic toxicity to fish, invertebrates or algae at concentrations up to the limit of solubility.

On the basis of the weight of evidence of the available data, a BCF of <10 and chronic NOEC of >125 mg/L, there are not considered to be sufficient grounds for concern for classifying branched hexatriacontane for chronic aquatic toxicity. As the as chronic toxicity NOECs are higher than the water solubility, it is proposed that the classification of chronic category 4 is removed from branched hexatriacontane.

6 OTHER INFORMATION

No other information is considered relevant to the proposed classification change.

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8 ANNEXES

Branched hexatriacontane (1-Dodecene trimer, hydrogenated) is a poly alpha olefin (PAO). PAO substances are highly branched iso-paraffinic chemicals produced by oligomerization of oct-1-ene, dec-1-ene, and/or dodec-1-ene. Therefore, their physiochemical and toxicological properties are expected to be similar. The majority of the PAO category members are phase-in substances and registered under REACH. Branched hexatriacontane is a NONS substance and not registered together with other PAO category members under REACH. Nevertheless, it falls within the applicability domain of the PAO category. Therefore, it is appropriate to use PAO category data for read across to branched hexatriacontane. Poly Alpha Olefin category members are all of the same hydrocarbon class. The hydrogenated materials are saturated hydrocarbons with some branching. The primary difference between category members is the carbon number range.

8.1 Read across from members of the poly alpha olefins category

The HOPA (Higher Olefins and Poly Alpha Olefins) REACH Consortium's Poly Alpha Olefins (PAO) category members are branched iso-paraffinic chemicals produced by polymerization/oligomerization of alpha olefins (e.g. 1-decene, 1-dodecene and 1-tetradecene), with the carbon number range typically from C20 to C60 and which may be hydrogenated.

Branched hexatriacontane comprises a mixture of branched C36 alkanes derived from 1-dodecene feedstock and therefore, although branched hexatriacontane was not registered as part of this category, it would clearly fall within the category domain. Data have been read across to branched hexatriacontane from the following substances within the HOPA REACH Consortium's Poly Alpha Olefin category.

Table 12: Poly alpha olefin substances used for read across

Name	CAS number	Carbon chain
Dec-1-ene, dimers, hydrogenated	68649-11-6	C20
1-decene dimer with dodecene, hydrogenated	151006-58-5	C22-24
1-Tetradecene, polymer with 1-dodecene, distn., residues, hydrogenated, C24-84 fraction	883233-93-0	C24-84
1-decene trimer, hydrogenated and tetramers	68649-12-7	C30-40
1-decene, homopolymer, hydrogenated	68037-01-4	C30-60
1-Dodecene polymer with 1-Decene, hydrogenated	151006-60-9	C30-84

Applicability

The HOPA REACH Consortium's Poly Alpha Olefin category applies to products that are made by the polymerization/oligomerization of alpha olefins. Category members are all of the same hydrocarbon class. The hydrogenated materials are saturated hydrocarbons with some branching. The primary difference between category members is the carbon number range. The poly alpha olefins are chemical intermediates with performance characteristics that are specific to the manufacturer/registrant. The polymerization process that occurs during the manufacturing process can affect the physical properties of a substance, which is why products may be registered under the same substance name and/or CAS number, but have different physical chemical properties including viscosity.

The Poly Alpha Olefins category covers products that are made from the polymerization/ oligomerization of alpha olefins (e.g. 1-decene, 1-dodecene and 1-tetradecene), with the carbon number range typically from C20 to C60, and includes hydrogenated materials which are saturated hydrocarbons with some branching. Branched hexatriacontane is a branched, saturated hydrocarbon, with a chain length of C36, derived from 1-dodecene feedstock. Therefore, branched hexatriacontane falls within the applicability domain of the poly alpha olefins category.

Hypothesis

The physico-chemical, fate and ecotoxicity properties of the poly alpha olefins are similar or change in a predictable fashion. For example, the water solubility is expected to decrease as the carbon number increases and the low water solubility of these hydrocarbon products is expected to limit the bioavailability to aquatic organisms thus their aquatic toxicity (US EPA 2005). The ecotoxicity of poly alpha olefins with the same carbon number is expected to be similar as they are neutral organic hydrocarbons which act via non-polar narcosis. Toxicity is due to the uptake of the chemical (proportional to log Kow) and then disruption of the function of biological membranes (US EPA 2005). It is therefore expected that poly alpha olefin products within the described carbon number range will behave in a similar manner and that use of read-across between members of the poly alpha olefins category and branched hexatriacontane is valid.

Justification

Poly Alpha Olefin category members are all of the same hydrocarbon class. The hydrogenated materials are saturated hydrocarbons with some branching and the primary difference between category members is the carbon number range, which typically ranges from C20 to C60. Branched hexatriacontane is a branched, saturated hydrocarbon, with a chain length of C36, derived from 1-dodecene feedstock. Therefore, branched hexatriacontane falls within the applicability domain of the poly alpha olefins category.

Branched hexatriacontane and the other poly alpha olefins category members are all of the same hydrocarbon class. The physico-chemical and environmental fate properties of the poly alpha olefins change in a predictable fashion, as can be observed in the results presented in Table 13. The melting point and boiling point increase with increasing chain length as the vapour pressure decreases. The water solubility decreases with increasing chain length and inversely, the log Kow, and therefore also the log Koc, increases. The half-life of the poly alpha olefins increases as the chain length increases, with the longer chain length substances, including branched hexatriacontane, showing limited biodegradation. The BCF of the poly alpha olefins increases initially, with a maximum value of 3362 L/kg at C16, then decreases with increasing chain length with the low water solubility limiting the bioavailability to aquatic organisms.

The partition coefficient results for the poly alpha olefins estimated using QSAR models gives a log Kow of ≥7.86 for C14 and above using the PETROTOX model and ≥7 for C14 and above (≥8 for C16 and above) using the ECOSAR model. Branched hexatriacontane, with a chain length of C36, is modelled have a log Kow of ≥8, which is supported by the experimental data available for this substance (log Kow ≥8). The water solubility results for the poly alpha olefins estimated using QSAR models gives a water solubility of ≤0.0139 mg/L for C14 and above using the ECOSAR model. Branched hexatriacontane, with a chain length of C36, is therefore modelled have a water solubility value of ≤1.16 E^{-10} mg/L, which is supported by the experimental data available for this substance (water solubility <0.482 mg/L).

ECOSAR and PETROTOX models were run for poly alpha olefins for C14 to C30 (see Table 13). The ecotoxicity effects of the poly alpha olefins change in a predictable fashion. The PETROTOX model shows no effects at the limit of solubility for poly alpha olefins of C14 and above. The

ECOSAR model shows an increase in aquatic toxicity with chain length, however as the water solubility decreases with chain length, from C30 and above, aquatic ecotoxicity effects are not observed below the water solubility. At chain lengths of C14 and above for PETROTOX, all ecotoxicity results showed no effects at >1000 mg/L and, at chain lengths of C30 and above for ECOSAR, all ecotoxicity results showed no effects at >1000 mg/L. Therefore, the results are not presented for poly alpha olefins of longer chain lengths, as all the results would be the same. The low water solubility of these hydrocarbon products limits the bioavailability to aquatic organisms and as toxicity is due to the uptake of the chemical (proportional to log Kow), poly alpha olefins of C30 and above show no toxicity to aquatic organisms at their limit of solubility. Therefore, branched hexatriacontane, with a chain length of C36, is modelled have no toxicity at the limit of solubility, which is supported by the experimental data available for this substance.

Conclusion

Branched hexatriacontane and the other poly alpha olefins category members are all neutral organic hydrocarbons which act via non-polar narcosis, though the low water solubility of these hydrocarbon products limits the aquatic toxicity. The aquatic toxicity results are presented in the IUCLID dossier and discussed in the sections above and in the appendix below. The data show that, for branched hexatriacontane, aquatic toxicity is not observed at loading concentrations far in excess of the water solubility (<4.82 $x10^{-4}$ g/L at 20°C). No effects were observed at the highest concentrations tested, with NOEC of >1000 mg/L, for acute toxicity to fish and invertebrates and acute and chronic toxicity to algae. The findings are further confirmed by both PETROTOX and ECOSAR QSAR models, which predict acute LC50 and chronic NOEC of >1000 mg/L and > water solubility, respectively, for fish, invertebrates and algae.

The data for poly alpha olefins show that aquatic toxicity is not observed at the highest concentrations tested (loading concentrations far in excess of the water solubility). In the acute studies, the highest concentration tested was 1000 mg/L for acute toxicity to fish, invertebrates and algae. In addition, a NOEC of >125 mg/L (highest concentration tested) was determined for chronic toxicity to aquatic invertebrates. Branched hexatriacontane has a typical carbon number of C36 and acute and chronic ecotoxicity data are presented for poly alpha olefins with a range of carbon numbers covering C36. The results read across from poly alpha olefins are presented in the following tables. Substances in the category for which data are not available have not been included in the tables.

Given the similarity in the toxicity results between branched hexatriacontane and members of the poly alpha olefins category for acute toxicity to fish and invertebrates and acute and chronic toxicity to algae, it is not expected that there would be any difference in the effects for chronic toxicity to invertebrates. As the substances are all of the same hydrocarbon class which has very low solubility and acts via non-polar narcosis, read across of the ecotoxicity data between branched hexatriacontane and other poly alpha olefins is considered to be justified.

Table 13: Summary of QSAR results on physico-chemical and environmental fate properties of poly alpha olefins of C14 and above

Endpoint	Program	Units	C14	C16	C18	C20	C22	C24	C30	C36
Melting point	MPBPVP (v1.43)	°C	0.41	21.29	29.57	50.38	70.75	96.76	150.9	187.08
Boiling point		°C	248.65	275.88	306.27	333.05	356.76	379.97	449.59	506.09
Vapour pressure		Pa	6.3	1.02	0.347	0.0545	0.0115	0.00153	9.50E-06	1.64E-07
Water solubility	WskowWin	mg/L	0.0139	0.00123	0.000126	1.26E-05	1.26E-06	1.24E-07	1.16E-10	1.02E-13
	WATERNT (v1.01)		0.00887	0.0004	3.79E-05	3.55E-06	3.30E-07	3.37E-07	4.21E-07	5.07E-07
Log Kow	KowWin	-	7	8.06	9.04	10.03	11.01	11.99	14.94	17.87
Log KOC - MCI	KOCWIN (v2.00)	-	4.204	4.726	5.247	5.768	6.289	6.811	8.375	9.848
Log KOC - Kow			6.0749	6.9949	7.8454	8.7046	9.5552	10.4057	12.966	15.509
BCF	BCFBAF (v3.01)	L/kg w.w.	3362	1016	335.4	110.7	36.56	12.07	3.162	3.162
HLC - Bond method	HENRYWIN (v3.20)	Pa-m^3/mole	4.14E+05	6.18E+05	1.09E+06	1.92E+06	3.38E+06	5.96E+06	3.26E+07	8.50E+08
HLC - Group method			5.95E+05	1.71E+06	3.42E+06	6.83E+06	1.36E+07	2.72E+07	2.16E+08	7.84E+09
Half-life	BioHCwin (v1.01)	days	8.846	17.23	23.39	31.75	43.11	58.53	146.5	474.5

Table 14: Summary of QSAR results on partition coefficient and ecotoxicity properties of poly alpha olefins of C14 and above

Variable/ Organism	Endpoint		≥C14	C14	C16	C18	C20	C22	C24	C30
	ECOSAR	PETROTOX	PETROTOX	ECOSAR	ECOSAR	ECOSAR	ECOSAR	ECOSAR	ECOSAR	ECOSAR
Log Kow			≥7.86	7	8.06	9.04	10.03	11.01	11.99	14.94
Water solubility				0.0139	0.00123	0.0001256	1.26E-05	1.26E-06	1.24E-07	1.16E-10
Fish	96h LC50	LL50	>1000^	0.006	0.000801	0.000123	1.87E-005 *	2.81E-006 *	4.19E-007 *	1.34E-009 *
Daphnid	48h LC50	LL50	>1000^	0.007	0.00111	0.000197*	3.46E-005 *	6.01E-006 *	1.04E-006 *	5.11E-009 *
Green Algae	96h EC50	LL50	>1000^	0.030*	0.007*	0.00199*	0.000536 *	0.000143 *	3.77E-005 *	6.69E-007 *
Fish	NOEC	NOEL	>1000	0.000876	0.000125	2.06E-05	3.34E-06	5.36E-07	8.53E-08	3.32E-010 *
Daphnid	NOEC	NOEL	>1000	0.00182	0.000335	6.96E-05	1.43E-005 *	2.9E-006 *	5.85E-007 *	4.6E-009 *
Green Algae	NOEC	NOEL	>1000	0.026*	0.008*	0.002*	0.00078 *	0.000245 *	7.61E-005 *	2.21E-006 *

* Chemical may not be soluble enough to measure this predicted effect.

^ LL50 not reached.

Table 15: Summary of relevant information on biodegradation and short-term ecotoxicity properties of poly alpha olefins

Name	C No.	Short-term fish	Short-term invert	Short-term algae	Biodegradation
Branched hexatriacontane – 1-Dodecene trimer, hydrogenated (CAS 151006-62-1)	C36	96 hr LC50 (nominal loading rate): >1000 mg/L (Handley 1995) GLP, K1, WAF, OECD 203 - *Oncorhynchus mykiss*, static, freshwater, based on mortality	48 hr EC50 (nominal loading rate): >1000 mg/L (Handley 1995) GLP, K1, WAF, OECD 203 - *Daphnia magna*, static, freshwater, based on mortality	96 hr EC50 (nominal loading rate): >1000 mg/L (Handley 1995) GLP, K1, WAF, OECD 201 - *Selenastrum capricornutum*, static, freshwater, based on biomass and growth rate	Not readily biodegradable - 19% (Mead 2005) GLP, K1, OECD 301B, aerobic, 28 days, domestic non-adapted activated sludge, 11.7 mg/L test item (nominal loading rate)
Poly alpha olefins C14+ ^	C14+	96 hr LC50: >1000 mg/L (DiToro 2010) QSAR, K2, PETROTOX model - *Oncorhynchus mykiss*, based on mortality	48 h LC50: >1000 mg/L (DiTorro 2010) QSAR, K2, PETROTOX model - *Daphnia magna*, based on mortality	72 h EC50: >1000 mg/L (DiTorro 2010) QSAR, K2, PETROTOX model - *Pseudokirchneriella subcapitata*, based on mortality	-
Poly alpha olefins ^	Log Kow >8*	96 hr LC50: >water solubility (Nabholz 2009) QSAR, K2, ECOSAR model – *fish*, based on mortality	48 hr LC50: >water solubility (Nabholz 2009) QSAR, K2, ECOSAR model - *Daphnia magna*, based on mortality	96 hr EC50: >water solubility (Nabholz 2009) QSAR, K2, ECOSAR model - *green algae*, based on mortality	-
Poly alpha olefin category member: Dec-1-ene, dimers, hydrogenated (CAS 68649-11-6)	C20	96 hr LC50 (nominal loading rate): >1000 mg/L (Mattock 1995a) GLP, K2, WAF, OECD 203 -*Oncorhynchus mykiss*, freshwater, semi-static 96 hr LC50 (nominal loading rate): >5003 mg/L (Gross 1992b) GLP, K2, Oil-Water-Dispersion, OECD 203 - *Cyprinodon variegatus*, freshwater, static	48 hr EC50 (nominal loading rate): >1000 mg/L (Mattock 1995c) GLP, K2, WAF, OECD 202 - *Daphnia magna*, freshwater, static, based on mobility 96 hr EC50 (nominal loading rate): >5056 mg/L (Lorenzoni 1992) GLP, K2, WAF, Equivalent to OECD 202 - *Americamysis bahia*, marine, semi-static, based on mobility	72 hr EC50 (nominal loading rate): >1000 mg/L (Mattock 1995e) GLP, K2, WAF, OECD 201 - *Scenedesmus capricornutum*, freshwater, static, based on biomass and growth rate	Not readily biodegradable - 15% (Douglas 1993) GLP, K1, OECD 301D, aerobic, 28 days, activated sewage sludge, 2 mg/L test item (nominal loading rate)
Poly alpha olefin category member: 1-decene dimer with dodecene, hydrogenated (CAS 151006-58-5)	C22-24	96 hr LC50 (nominal loading rate): >1000 mg/L (Bowman 1989a) GLP, K1, WAF, EPA - 660/3-75-009 - *Oncorhynchus mykiss*,	48 hr EC50 (nominal loading rate): >150 mg/L (Forbis 1989) GLP, K2, WAF, EPA 797.1300 - *Daphnia magna*, freshwater, semi-static, based on mobility	96 hr EC50 (nominal loading rate): >1000 mg/L (Forbis 1990) GLP, K2,WAF, EPA 797.1050 - *Pseudokirchneriella subcapitata,* freshwater, static, based on cell number	Readily biodegradable, but failing 10-day window - 66% (Douglas 1989) GLP, K1, OECD 301D, aerobic, 28 days, non-adapted active sludge, 2 mg/L test item

Name	C No.	Short-term fish	Short-term invert	Short-term algae	Biodegradation
		freshwater, semi-static			(nominal loading rate)
Poly alpha olefin category member: 1-Tetradecene, polymer with 1-dodecene, distn., residues, hydrogenated, C24-84 fraction (CAS 883233-93-0)	C24-84	-	-	-	Not readily biodegradable – 54.3% (Hamwijk 2002) GLP, K2, OECD 301B, aerobic, 28 days, activated domestic sewage, 11.8-23.7 mg/L test item (nominal loading rate)
Poly alpha olefin category member: 1-decene trimer, hydrogenated and tetramers (CAS 68649-12-7)	C30-40	96 hr LC50 (nominal loading rate): >5002 mg/L (Gross 1992a) GLP, K2, Oil-Water-Dispersion, OECD 203 - *Cyprinodon variegatus*, freshwater, static	96 hr LC50 (nominal loading rate): >5002 mg/L (Lorenzoni 1993) GLP, K2, WAF, equivalent to OECD 202 - *Americamysis bahia*, marine, semi-static, based on mobility	-	Not readily biodegradable – 49.2-53.5% (Mehta 1992) K2,OECD 301B, aerobic, activated sewage sludge and soil, 28 days, 10 and 20 mg/L test item (nominal loading rate)
Poly alpha olefin category member: 1-decene, homopolymer, hydrogenated (CAS 68037-01-4)	C30-60	96 hr LC50 (nominal loading rate): >1000 mg/L (Bowman 1989b) GLP, K1, WAF, EPA-660/3-75-009 - *Oncorhynchus mykiss*, freshwater, semi-static 96 hr LC50 (nominal loading rate): >1000 mg/L (Mattock 1995b) GLP, K1, WAF, OECD 203 - *Oncorhynchus mykiss*, freshwater, semi-static	48 hr EC50 (nominal loading rate): >1000 mg/L (Mattock 1995d) GLP, K1, WAF, OECD 202 - *Daphnia magna*, freshwater, static, based on mobility 48 hr EC50 (nominal loading rate): >130 mg/L (Forbis 1988) GLP, K2, WAF, equivalent to US EPA - *Daphnia magna*, freshwater, static, based on mobility	72 hr EC50 (nominal loading rate): >1000 mg/L (Mattock 1995f) GLP, K2, WAF, OECD 201 - *Scenedesmus capricornutum*, freshwater, static, based on biomass and growth rate	Not readily biodegradable - 2% (Douglas 1993) GLP, K1, OECD 301D, aerobic, 28 days, activated sewage sludge bacteria, 2 mg/L test item (nominal loading rate)
Poly alpha olefin category member: 1-Dodecene polymer with 1-Decene, hydrogenated (CAS 151006-60-9)	C30-84	96 hr LC50 (nominal loading rate): >1000 mg/L (Handley 1995) GLP, K1, WAF, OECD 203- *Oncorhynchus mykiss*, freshwater, semi-static	48 hr EC50 (nominal loading rate): >1000 mg/L (Handley 1995) GLP, K1, WAF, OECD 202 - *Daphnia magna*, freshwater, static	-	Not readily biodegradable – 7% (Handley 1995) GLP, K2, OECD 301B, aerobic, 28 days, activated sewage sludge microorganisms, 20 mg/L DOC

* No carbon chain length is reported for the ECOSAR results as the QSAR uses the log Kow. For acute toxicity, empirical data indicate that, at log Kow values of greater than 5.0 for fish and invertebrates and 6.4 for algae, the decreased solubility results in “no effects at saturation”.

^ Standard test durations assumed.

Table 16: Overview of information on long-term aquatic toxicity of poly alpha olefins

Name	C number	Long-term fish	Long-term invert	Long-term algae
Branched hexatriacontane – 1-Dodecene trimer, hydrogenated (CAS 151006-62-1)	C36	-	-	96 hr NOEC (nominal loading rate): ≥1000 mg/L (Handley 1995) GLP, K1, WAF, OECD 201 - *Selenastrum capricornutum*, static, freshwater, based on biomass and growth rate
Poly alpha olefins C14+ ^	C14+	30 d NOEC: 1000 mg/L (DiTorro 2010) QSAR, K2, PETROTOX model - *Oncorhynchus mykiss*, based on mortality	21 d NOEC: 1000 mg/L (DiTorro 2010) QSAR, K2, PETROTOX model - *Daphnia magna*, based on mortality	72 h NOEC: 1000 mg/L (DiTorro 2010) QSAR, K2, PETROTOX model - *Pseudokirchneriella subcapitata*, based on mortality
Poly alpha olefins ^	Log Kow >8 *	30 d NOEC: >water solubility (Nabholz 2009) QSAR, K2, ECOSAR model - *fish*, based on mortality	21 d NOEC: >water solubility (Nabholz 2009) QSAR, K2, ECOSAR model - *Daphnia magna*, based on mortality	96 h NOEC: >water solubility (Nabholz 2009) QSAR, K2, ECOSAR model - *green algae*, based on mortality
Poly alpha olefin category member: Dec-1-ene, dimers, hydrogenated (CAS 68649-11-6)	C20	-	21 d NOEC (nominal loading rate): 125 mg/L (Putt 2003a) GLP, K1, WAF, OECD 211 - *Daphnia magna*, freshwater, semi-static, based on mortality, timing of first brood, number of offspring, length and weight	72 hr NOEC (nominal loading rate): 1000 mg/L (Mattock 1995e) GLP, K2, WAF, OECD 201 - *Scenedesmus capricornutum*, freshwater, static, based on biomass and growth rate
Poly alpha olefin category member: 1-decene dimer with dodecene, hydrogenated (CAS 151006-58-5)	C22-24	-	-	96 hr NOEC (nominal loading rate): 1000 mg/L (Forbis 1990) GLP, K2, WAF, EPA 797.1050 - *Pseudokirchneriella subcapitata,* freshwater, static, based on cell number
Poly alpha olefin category member: 1-decene, homopolymer, hydrogenated (CAS 68037-01-4)	C30-60	-	21 d NOEC (nominal loading rate): 125 mg/L (Putt 2003b) GLP, K1, WAF, OECD 211 - *Daphnia magna*, freshwater, semi-static, based on mortality, timing of first brood, number of offspring, length and weight	72 hr NOEC (nominal loading rate): 1000 mg/L (Mattock 1995f) GLP, K2, WAF, OECD 201 - *Scenedesmus capricornutum*, freshwater, static, based on biomass and growth rate

***** No carbon chain length is reported for the ECOSAR results as the QSAR uses the log Kow of category members. For chronic toxicity, log Kow values of greater than 8 indicate that the decreased solubility results in "no effects at saturation".

^ Standard test durations assumed.

A data matrix of the aquatic toxicity data is presented according to the number of carbon atoms in the substance to demonstrate the lack of toxicity of a range of poly alpha olefins, including branched hexatriacontane (C36), to aquatic organisms.

Table 17: Overview of information on aquatic toxicity of poly alpha olefins

			LC/EC50 (acute) or NOEC (chronic) mg/L for carbon number																				
			20	22	24	26	28	30	32	34	**36**	38	40	42	44	46	48	50	52	54	56	58	60
fish	acute	experimental	>1000																				
			>5003																				
			>1000																				
								>5002															
											>1000												
								>1000															
								>1000															
								>1000															
		modelled	> water solubility (Ecosar) and >1000 (Petrotox)																				
	chronic	experimental																					
		modelled	> water solubility (Ecosar) and >1000 (Petrotox)																				
invertebrates	acute	experimental	>1000																				
			>5056																				
			>150																				
								>5002															
											>1000												
								>130															
								>1000															
								>1000															
		modelled	> water solubility (Ecosar) and >1000 (Petrotox)																				
	chronic	experimental	125																				
								125															
		modelled	> water solubility (Ecosar) and >1000 (Petrotox)																				
algae	acute	experimental	>1000																				
			>1000																				
								>1000															
		modelled	> water solubility (Ecosar) and >1000 (Petrotox)																				
	chronic	experimental	1000																				
			1000																				
								1000															
		modelled	> water solubility (Ecosar) and >1000 (Petrotox)																				

Green highlighting indicates no acute or chronic toxicity observed in the experimental study or QSAR prediction.
Grey highlighting indicates the carbon number of branched hexatriacontane.