

Category B 'Butylene Oligomers- Chemical Category Justification

(NB : all compositions are in w/w for liquids and v/v for gases)

| Category definition and its members | | | | | | | | | | | | | | | | | |
|--|---|--|------------|----------------------|---------------------------|------------|--------------------------------|---------------------------------|------------|---|-------------------------|-----------|--------------------------|------------------------|-----------|---|--|
| 1.1. | Category Definition | | | | | | | | | | | | | | | | |
| 1.1.a. | Category Hypothesis | | | | | | | | | | | | | | | | |
| <p>Butylene Oligomers category contains hydrocarbon streams obtained by the oligomerisation of butylenes. The substances within this category consist predominantly of C4, C8, C12, C16 and/or C20 hydrocarbons. The category stream components boil between 30 and 350 °C and the streams contain less than 0.1% butadiene.</p> <p>It is reasonable to assume that the phys-chem and environmental fate properties of the category members will be similar and likely to change in a relatively uniform manner, as the carbon number increases consistently. The streams should demonstrate a trend with respect to environmental effects as the constituents will act via narcosis, until a solubility cut-off is reached, at which point no toxicity will be observed. With regard to mammalian endpoints, category members are liquids of moderate volatility with inhalation and skin contact representing probable routes of exposure. CNS depression and/or skin irritation (marker substance: dodecene, branched) are likely to be the predominant health hazards. Long-term irreversible effects are not anticipated. It can therefore be assumed that streams meeting the applicability domain will behave in a similar, or demonstrate a trend, depending upon the end-point, and that the use of read-across is valid. As the 1,3-butadiene content of the streams is less than 0.1% w/w for all category members they will not be impacted by any classification or hazard assessment based on butadiene as a constituent.</p> | | | | | | | | | | | | | | | | | |
| 1.1.b. | Applicability domain (AD) of the category | | | | | | | | | | | | | | | | |
| <p>The category contains streams that are composed of butylene sub-units with less than 0.1% butadiene.</p> <p>Specific components (The range entered below is that currently based on received analytical data, it is not intended to be prescriptive. See section 1.3).</p> <p><i>1,3-butadiene - <0.1%</i></p> <p>PIONA* :</p> <p>Olefins - >95% - C8 - >C20</p> <p><i>*: PIONA refers to a description of the type of hydrocarbons present, paraffins, isoparaffins, olefins, naphthenics (cycloparaffins) and aromatics. It does not refer to a specific type of analysis or determination.</i></p> | | | | | | | | | | | | | | | | | |
| 1.2. | Category Members | | | | | | | | | | | | | | | | |
| <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="width: 20%; padding: 5px;">CAS Number</th> <th style="width: 40%; padding: 5px;">Official Description</th> <th style="width: 40%; padding: 5px;">Registered Substance Name</th> </tr> </thead> <tbody> <tr> <td style="text-align: center; padding: 5px;">42278-27-3</td> <td style="padding: 5px;">1-Propene, 2-methyl-, pentamer</td> <td style="padding: 5px;">1- propene, 2-methyl-, pentamer</td> </tr> <tr> <td style="text-align: center; padding: 5px;">68606-29-1</td> <td style="padding: 5px;">Hydrocarbons, C4 and C8, butene concentrator by-product</td> <td style="padding: 5px;">Dimers (di isobutylene)</td> </tr> <tr> <td style="text-align: center; padding: 5px;">7756-94-7</td> <td style="padding: 5px;">2-Methylpropene, trimers</td> <td style="padding: 5px;">Methylpropene, trimers</td> </tr> <tr> <td style="text-align: center; padding: 5px;">9003-29-6</td> <td style="padding: 5px;">Butene, homopolymer (products derived from either/or But-1-ene/But-2-ene)</td> <td style="padding: 5px;">Butene, homopolymer (products derived from either/or But-1-ene/But-2-ene) Consisting of 50 wt % or more of species of the same M.Wt</td> </tr> </tbody> </table> | | | CAS Number | Official Description | Registered Substance Name | 42278-27-3 | 1-Propene, 2-methyl-, pentamer | 1- propene, 2-methyl-, pentamer | 68606-29-1 | Hydrocarbons, C4 and C8, butene concentrator by-product | Dimers (di isobutylene) | 7756-94-7 | 2-Methylpropene, trimers | Methylpropene, trimers | 9003-29-6 | Butene, homopolymer (products derived from either/or But-1-ene/But-2-ene) | Butene, homopolymer (products derived from either/or But-1-ene/But-2-ene) Consisting of 50 wt % or more of species of the same M.Wt |
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| | | |
|------------|--|--|
| | | butene, homopolymer |
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| 91052-99-2 | Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction | Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction |
| 91053-00-8 | Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutylene fraction | Hydrocarbons, C4, 1,3-butadiene-free, polymd., tetraisobutylene fraction |
| 91053-01-9 | Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction | Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction |
| 93685-78-0 | Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated | Hydrocarbons, C4, 1,3-butadiene-free, polymd., dibutylene fraction, hydrogenated |
| 97280-83-6 | Trimer of Butenes | Isododecene |

1.3. Purity / Impurities

The substances in this category are UVCBs and as such are considered to be 100% pure. The term impurity is not relevant for UVCBs, however, substances will be described using the following:

- Known constituents present at 10% or greater (if any), identified by IUPAC name and EC number/CAS number, indicating typical concentrations and/or concentration ranges;
- Constituents relevant for hazard classification (if any);
- Constituents relevant for PBT assessment (if any).

2. Category justification

Butylene Oligomers category contains hydrocarbon streams obtained by the oligomerisation of butylenes. The substances within this category consist predominantly of C4, C8, C12, C16 and/or C20 hydrocarbons. The category stream components boil between 100 and 350 °C and the streams contain less than 0.1% butadiene. The physico-chemical properties associated with these types of UVCBs indicated that they comprise a category based on the range of boiling points (from 30°C to 350°C) and will have similar behaviour in the environment. The estimated log Kow ranges from 4.12-9.91 and the streams in this category are considered to be readily biodegradable. The mammalian toxicity information and environmental assessment also indicated that the streams in this category exert similar effects.

3. Data matrix

Butylene Oligomers is a UCVB category and therefore identification of trends between category members is not appropriate and therefore, according to the ECHA Guidance on information requirements and chemical assessment Chapter R.6, it is not feasible to establish a full data matrix for this category. Consequently, a data set that applies to all members of this category has been developed.

4. Conclusions per endpoint for C&L, PBT/vPvB and dose descriptor

CLASSIFICATION AND LABELLING

Physico-chemical Hazard Assessment

- **Boiling point** - The measured boiling point of streams in this category is in the range 109.8°C to 202°C. An agreed range for this category was determined to be 30°C to 350 °C.

- **Partition coefficient** - The streams in this category have estimated partition coefficients ranges from log Kow 4.12-9.91.
- **Flash point** - The flash point of streams in this category is 71 °C. Due to the high flashpoint this category is not classified for flammability.

Human Health Hazard Assessment

- **Toxicokinetics** – Data available on higher olefins similar to those found in the butylene oligomer category suggest that metabolism occurs in hepatic endoplasmic reticulum via initial formation of a transient epoxide, which is further metabolized to the corresponding glycol or conjugated with glutathione. Following oral or inhalation exposure, these higher olefins can be absorbed into the blood and reach the liver and kidneys
- **Acute toxicity** – Acute toxicity studies exist for higher olefins including butylene oligomers at both ends of the carbon number ranges within this category. The results are consistent throughout the category and indicate low acute toxicity by the oral, dermal and inhalation routes of exposure. Butylene oligomers have low kinematic viscosity.
- **Irritation** – Tetrabutene (mixture of C16 and C20 olefin isomers) was found to be non irritating to the skin. However C8 and C12 butylene oligomers using occlusive dressings were found to be irritating to rabbit skin. In a study where a semi occlusive dressing was used, 2,4,4, TMP (a C8 olefin) was found to be non-irritating. However another C8 substance, diisobutylene was found to be moderately irritating to rabbit skin using semi-occlusive conditions. In four representative studies it was found that the test materials were not irritating to the rabbit eye. There are no specific studies on respiratory tract irritation but there was no evidence of respiratory tract irritation in a 90 day inhalation with isooctene.
- **Sensitisation** – Not skin or respiratory sensitisers
- **Repeat dose toxicity** – There is a 28 day repeat oral dosing study with triisobutylene with 14 day recovery. There are also repeat dose toxicity studies with other higher olefins spanning the range C8 to C20. The data for these studies indicate that the location of the double bond or the addition of branching to the structure do not appear to affect the toxicity. Higher olefins are of low toxicity in rats. Male rat kidney effects indicative of alpha-2u-globulin nephropathy consistently occur with the C8 to C14 higher olefins. Alpha-2u-globulin nephropathy is considered to be male rat-specific and is not relevant for humans. Treatment-related liver effects (increased organ weights, hepatocyte cytoplasmic vacuolation, and centrilobular hepatocyte hypertrophy) are also observed in rats exposed to higher olefins, which may reflect adaptive changes as a result of the high liver burden of these substances. There is no evidence of neurotoxicity.
- **Genetic toxicity** – There is no evidence of mutagenicity in vitro or in vivo in a range of recognised core assay types conducted with butylene oligomers or representative olefins. In vitro studies comprise six bacterial reverse mutation assays with olefins ranging from C8 to C20/24 and two mammalian chromosome aberration tests with C8. There are also four negative in vivo mammalian erythrocyte micronucleus tests in the mouse or the rat covering three different routes of administration oral, inhalation and intraperitoneal and olefins ranging from C8 to C20/C24. The results are consistent throughout the category.
- **Carcinogenicity** – On the basis of the available evidence it can be concluded that butylene oligomers are not genotoxic and are unlikely to be carcinogenic.
- **Toxic to reproduction** – There are sufficient data available on representative substances to

conclude that members of the butylenes oligomers category are unlikely to have effects on reproduction, fertility or offspring development and do not warrant classification

Environmental Hazard Assessment

- **Biodegradation** - Based on one experimental study the streams in this category have been shown to be readily biodegradable and will be considered readily biodegradable
- **Bioaccumulation** - Log BCF have been calculated for various representative components of these streams. The calculated values range from 2.8-4.5.
- **Ecotoxicity** - Four toxicity studies are available for acute invertebrate, algal and fish toxicity for the streams 97280-83-6 and 9003-29-6. The reported effect concentrations were based on WAF data and the ranged from >1.55 - >100mg/l WAF.

Based on the results of the hazard assessment the streams in this category would not be classified for environmental effects.

CONCLUSION FOR PBT

The screening assessment of the available data indicates that the properties of the members of this category do not meet the specific criteria detailed in Annex XIII or do not allow a direct comparison with all the criteria in Annex XIII but nevertheless indicate that the substance would not have these properties and therefore are not considered PBT/vPvB.

CONCLUSION FOR DOSE DESCRIPTOR

Environment: Deriving PNECs for UVCB substances based on WAF information is inappropriate. As the substance is a hydrocarbon UVCB the hydrocarbon block method has been used for environmental risk assessment (see REACH guidance, R7, app.13-1). The Petrorisk model (Redman, A. (2010). PETRORISK Users Guide, HydroQual, Inc., for Conservation of Clean Air and Water in Europe (CONCAWE)), was used for the environmental assessment. Blocks of C4-C20 carbon atoms and with a boiling point range of 108.9 °C to 350 °C were used in the modelling exercise. The model assigns individual structures from the library to the hydrocarbon blocks that the user enters. The input parameters are provided in Appendix B of the CSR. Details of the library structure mapping, some relevant physico-chemical properties and the mass fraction that is assigned to each chemical are also found in this appendix.

Human Health:

No DNELs were developed since no adverse treatment-related effects of relevance to humans were apparent from the underlying data.