

### Category L 'Resin oils and cyclic dienes' - Chemical Category Justification

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

<b>Category definition and its members</b>	
<b>1.1.</b>	<b>Category Definition</b>
<b>1.1.a.</b>	<b>Category Hypothesis</b>
<p>The <b>Resin oils and cyclic dienes</b> category covers hydrocarbons typically produced by the distillation of products from a steam cracking process. Imported streams will need to confirm that they meet the chemical description and are in domain. The category contains non-hydrotreated products (the Resin Oil products) and two products that are concentrates (1) dicyclopentadiene (DCPD) and (2) methylcyclopentadiene dimer (MCPD). Member of this category will have a carbon number distribution that is predominantly C5 – C15 and may contain more than 0.1 % isoprene and/or more than 0.1% benzene or 1,3-butadiene. Companies importing streams will need to confirm that such streams meet the chemical description and are in domain.</p> <p>By definition, from the category, these streams have overlapping hydrocarbon compositions, within a defined range, and hence, will have similar properties. It is therefore reasonable to assume that the components of the category will behave in a reasonably predictable manner, and with respect to phys-chem and environmental fate and effect properties read-across is valid</p> <p>For mammalian endpoints, the predominant route of exposure will be by inhalation and in those streams that contain benzene, butadiene and isoprene these will be the major drivers for effects.</p> <p>For mammalian endpoints, the classification of these streams will be driven by the content of benzene, 1,3-butadiene or isoprene when more than 0.1%, by the content of naphthalene when more than 1%, and by the content of toluene when more than 5%.</p>	
<b>1.1.b.</b>	<b>Applicability domain (AD) of the category</b>
<p>The category applies to streams with the following PIONA* analysis: predominantly (iso)paraffins, olefins, naphthenics and aromatics and a carbon number range of predominantly 5-15, some streams will contain more than 0.1% isoprene, benzene, 1,3-butadiene, naphthalene and/or toluene.</p> <p><i>Boiling Point –the streams in this category will boil predominantly in the range of 100 - 220°C</i></p> <p><b>Specific components</b> (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>Benzene: &lt;0.1 – 40%</i></p> <p><i>1,3-butadiene: &lt;0.1 – 1%</i></p> <p><i>Isoprene : &lt;0.1 to 3%</i></p> <p><i>Toluene: up to 22%</i></p> <p><i>Naphthalene: up to 48%</i></p> <p><i>Styrene: up to 40%</i></p> <p><i>C8 Aromatics (xylenes, ethylbenzene): up to 25%</i></p> <p><b>PIONA* :</b></p> <p>(iso)Paraffins – up to 50% : C# 4 - 12</p> <p>Olefins – up to 60% : C# 5 - 15</p>	

Naphthenics – up to 90% : C# 5 - 15

Aromatics – up to 100% : C# 5 – 15

\*: PIONA refers to a description of the type of hydrocarbons present, paraffins, isoparaffins, olefins, naphthenics and aromatics. It does not refer to a specific type of analysis or determination.

**1.2. Category Members**

CAS Number	CAS Description	Registered Substance Name
101316-62-5	Extract residues (coal), light oil alk., acid ext., indene fraction	Distillates (petroleum), alkene-alkyne manufact. pyrolysis oil, naphthalene fraction
102110-15-6	Hydrocarbons, C5-rich, dicyclopentadiene-contg.	Hydrocarbons, C5-rich, dicyclopentadiene-contg
		Raw Piperylene
65996-79-4	Solvent naphtha (coal)	Solvent naphtha (coal)
68477-40-7	Distillates (petroleum), cracked stripped steam-cracked petroleum distillates, C10-12 fraction	Distillates (petroleum), cracked stripped steam-cracked petroleum distillates, C10-12 fraction
68477-50-9	Distillates (petroleum), polymd. steam-cracked petroleum distillates, C5-12 fraction	C5 Raffinate
68477-53-2	Distillates (petroleum), steam-cracked, C5-12 fraction	Distillates (petroleum), steam-cracked, C5-12 fraction
68477-54-3	Distillates (petroleum), steam-cracked, C8-12 fraction	Distillates (petroleum), steam-cracked, C8-12 fraction
		Aromatic HCD C9
68478-10-4	Naphtha (petroleum), light steam-cracked, debenzenized, C8-16-cycloalkadiene conc.	CPD-DCPD cyclics
68516-20-1	Naphtha (petroleum), steam-cracked middle arom.	Naphtha (petroleum), steam-cracked middle arom.
		Xylene rich
68526-56-7	Alkenes, C9-11, C10-rich	Alkenes, C9-11, C10-rich

68527-26-4	Naphtha (petroleum), light steam-cracked, debenzenized	Naphtha (petroleum), light steam-cracked, debenzenized
94733-07-0	Distillates (petroleum), cracked, ethylene manuf. by-product, C9-10 fraction	Distillates (petroleum), cracked, ethylene manuf. by-product, C9-10 fraction
<b>1.3.</b>	<b>Purity / Impurities</b>	
<p>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:</p> <ul style="list-style-type: none"> <li>○ <u>Known</u> constituents present at 10% or greater (if any), identified by IUPAC name and EC number/CAS number, indicating typical concentrations and/or concentration ranges;</li> <li>○ Constituents relevant for hazard classification (if any);</li> <li>○ Constituents relevant for PBT assessment (if any).</li> </ul>		
<b>2.</b>	<b>Category justification</b>	
<p>The <b>Resin oils and cyclic dienes</b> category covers hydrocarbons typically produced by the distillation of products from a steam cracking process. Imported streams will need to confirm that they meet the chemical description and are in domain. The category contains non-hydrotreated products (the Resin Oil products) and two products that are concentrates (1) dicyclopentadiene (DCPD) and (2) methylcyclopentadiene dimer (MCPD). Member of this category will have a carbon number distribution that is predominantly C5 – C15 and may contain more than 0.1 % isoprene and/or more than 0.1% benzene or 1,3-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 100°C to 220°C) and will have similar behaviour in the environment. The log Kow ranges from 2.2 to &gt;6.5 and the streams in this category are not considered to be readily biodegradable. The mammalian toxicity information and environmental assessment also indicated that the streams in this category exert similar effects.</p>		
<b>3.</b>	<b>Data matrix</b>	
<p><b>Resin oils and cyclic dienes</b> 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.</p>		
<b>4.</b>	<b>Conclusions per endpoint for C&amp;L, PBT/vPvB and dose descriptor</b>	
<b><u>CLASSIFICATION AND LABELLING</u></b>		
<b>Physico-chemical Hazard Assessment</b>		
<ul style="list-style-type: none"> <li>● <b>Boiling point</b> - The measured boiling point of streams in this category was ranged from 167°C to 193°C (agreed category boiling point ranged from 100°C to 220°C).</li> <li>● <b>Partition coefficient</b> - The streams in this category have partition coefficients ranges from log Kow 2.8 to &gt;6.5.</li> <li>● <b>Flash point</b> - The flash point of streams in this category is 44.5 °C to 76°C. Some streams will have the following classification.   <u>Flashpoint of ≥ 23 °C and initial boiling point ≤ 60 °C.</u>             Flam. Liquid 3 (Hazard statement: H226: Flammable liquid and vapour.</li> </ul>		

### Human Health Hazard Assessment

- **Toxicokinetics** – The marker substances for this category (benzene, 1,3-butadiene, isoprene, toluene, naphthalene, styrene and C8 aromatics), in their pure form, have well-defined toxicokinetic parameters that have been taken into account during the derivation of their respective DNEL's. The overall DNEL of this category is driven by the DNELs for benzene, naphthalene and styrene.
- **Acute toxicity** – Resin Oils and Cyclic Dienes streams are of low acute toxicity by the dermal route and do not warrant classification for this end-point. Some streams are hazardous following oral or inhalation exposure and streams containing  $\geq 25\%$  naphthalene will need to be classified for oral toxicity.
- **Irritation** – Resin Oils and Cyclic Dienes streams are considered to be skin and eye irritants. If the combined concentration of xylenes and ethylbenzene is  $\geq 10\%$  the stream is also considered to be a respiratory irritant.
- **Sensitisation** – Not sensitising.
- **Repeat dose toxicity** – The limited repeat dose toxicity data on specific streams identified for this category (oral toxicity studies for CAS 68477-54-3 [Low Dicyclopentadiene Resin Oil] and CAS 48478-10-4 [Dicyclopentadiene/Codimer Concentrate] provided no evidence of significant target organ toxicity. However, there are substantial data on the repeated dose toxicity of a number of specific components present in some streams which demonstrate significant target organ toxicity and when present at concentrations greater than or equal to 1% (benzene) or 10% (toluene, styrene and ethylbenzene) will drive the mammalian toxicity effects.
- **Genetic toxicity** – In vitro and in vivo genotoxicity data are available for 2 streams within this category - CAS 68477-54-3 (Low Dicyclopentadiene Resin Oil) and CAS 68478-10-4 (Dicyclopentadiene/Codimer Concentrate). These studies show negative results. However, data on the genotoxicity of the marker substances, benzene, 1,3-butadiene and isoprene show them to be mutagenic in vivo. Streams that contain  $\geq 0.1\%$  benzene or 1,3-butadiene or  $\geq 1\%$  isoprene are considered to be mutagenic and will require classification for this end-point.
- **Carcinogenicity** – There are no specific carcinogenicity data on any of the streams within this category. However, there are substantial data on the carcinogenicity of a number of specific components present in some streams. Of these, benzene, 1,3-butadiene, naphthalene and isoprene have been shown to be carcinogenic. Resin Oils and Cyclic Dienes are considered to be carcinogens if they contain  $\geq 0.1\%$  benzene, 1,3-butadiene or isoprene or  $\geq 1\%$  naphthalene.
- **Toxic to reproduction** – Limited reproduction toxicity data are available for 2 streams within this category (CAS 68477-64-3: Low Dicyclopentadiene Resin Oil; CAS 68478-10-4: Dicyclopentadiene/Codimer Concentrate). In OECD Guideline 422 studies no evidence of impaired fertility or teratogenicity was seen. For CAS 68477-54-3 (Low dicyclopentadine resin oil) lower pup body weight was seen at maternally toxic doses. Data on the reproductive and developmental toxicity of specific components present in some streams indicate that none possesses specific effects on fertility which warrant classification but toluene is labelled with respect to developmental toxicity. Therefore, classification and labelling with respect to developmental toxicity will be driven by the concentration of toluene in Resin Oils and Cyclic Dienes streams.

### Environmental Hazard Assessment

- **Biodegradation** - Based on two experimental studies the streams in this category have not been shown to be readily biodegradable and will not be considered readily biodegradable.

- **Bioaccumulation** - BCF have been calculated using for various representative components of these streams. Using a log Kow range of 2.68 to 6.96 the calculated values range from 26 to 18000. The latter figure was calculated for a C15 Olefin, all other BCF values for the category fall within the range 26-174.
- **Ecotoxicity** – The available studies for category members showed similar results across the three trophic levels. Two fish studies provided a 96 hr LL50 range between 0.73 – 6.3 mg/l (96 hr LC50 ranged from 0.58 – 58.6mg/l in 5 studies). Two invertebrate studies provided 48 hr EL50 range of 0.91 – 3.2 mg/l (48 hr EC50 ranged 0.76-2.9mg/l). Two 72 hr algae studies provided a 72 hr ErL50 range of 1.3-1.5 (72 hr ErC50 ranged 0.84-1.4 mg/l).

Based on the available experimental data streams in this category should have the classification R50/53 under the DSD and Acute 1 Chronic 1 under the CLP regulations.

### **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 C5-C15 carbon atoms and with a boiling point range of 100°C to 307.9 °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:**

In general, risk characterization will be based on the premise that a marker substance with a low DN(M)EL present at high concentration in a stream will possess a greater relative hazard potential than a marker substance with a higher DN(M)EL present at the same or lower concentration.

Against this background, the most hazardous marker substances present in these streams are highlighted in the following table:

### Workers

Marker substance	Indicative concentration (%)	Inhalation		Dermal	
		DN(M)EL mg/m <sup>3</sup>	Relative hazard potential (max % ÷ DN(M)EL)	DN(M)EL mg/kg bw/d	Relative hazard potential (max % ÷ DN(M)EL)
benzene	<0.1 to 40	3.25	12.3	23.4	1.71
1,3-butadiene	<0.1 to 1	2.21	0.45	na	na
isoprene	<0.1 to 3	8.4	0.36	23.7	0.13
toluene	Up to 22	192	0.11	384	0.06
naphthalene	Up to 48	50	0.96	72	0.67

styrene	Up to 40	17	2.35	60	0.67
xylenes	Up to 25	221	0.11	3182	<0.01
ethylbenzene	Up to 25	77	0.32	180	0.14

Based on this analysis, demonstration of “safe use” for inhalation and dermal hazards associated with the presence of benzene will also provide adequate protection for workers against hazards arising from other marker substances present.

General population

Marker substance	Indicative concentration (%)	Inhalation		Dermal		Oral	
		DN(M)EL mg/m <sup>3</sup>	Relative hazard potential (max % ÷ DN(M)EL)	DN(M)EL mg/kg bw/d	Relative hazard potential (max % ÷ DN(M)EL)	DN(M)EL mg/kg bw/d	Relative hazard potential (max % ÷ DN(M)EL)
benzene	<0.1 to 40	<i>supply of streams containing ≥0.1% benzene prohibited</i>					
1,3-butadiene	<0.1 to 1	<i>supply of steams containing ≥0.1% butadiene prohibited</i>					
isoprene	<0.1 to 3	8.4	0.36	71	0.04	0.21	14.3
toluene	Up to 22	56.5	0.39	226	0.10	8.13	2.71
naphthalene	Up to 40	14.7	3.26	42.4	1.13	4.23	11.2
styrene	Up to 40	10.2	3.92	343	0.12	2.1	19.0
xylenes	Up to 25	65.3	0.38	1872	0.01	12.5	2.00
ethylbenzene	Up to 25	14.8	1.69	108	0.23	1.60	15.6

For the general population the long term inhalation and oral DNELs for styrene and long term dermal DNEL for naphthalene will be used for risk characterization.