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**US Environmental Protection Agency  
High Production Volume Chemical Challenge Program**

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**Category Summary  
for  
Higher Olefins Category**

**Prepared by:  
Higher Olefins Panel of the American Chemistry Council**

**April 28, 2005**

### SUMMARY CONCLUSIONS FOR HIGHER OLEFINS CATEGORY

The Higher Olefins Panel of the American Chemistry Council (ACC) hereby submits the category summary report for the Higher Olefins Category under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program.

#### Category Rationale

Due to similarities of this non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins ( $C_6$  through  $C_{54}$ ) under 30 CAS numbers (13 for alpha olefins and 17 for internal olefins), a category approach was utilized. All CAS numbers are within the EPA's HPV Chemical Challenge Program. The  $C_6 - C_{14}$  even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Higher Olefins Panel sponsored the  $C_6, C_7, C_8, C_9, C_{10}, C_{12}$  and  $C_{10-13}$  predominantly linear internal olefins and the  $C_{16}$  and  $C_{18}$  linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). For the purposes of the EPA HPV Chemical Challenge Program, the category was defined as "Higher Olefins." The category designation was based on the belief that, within the  $C_6$  to  $C_{54}$  boundaries identified, internalizing the location of the carbon-carbon double bond, increasing the length of the carbon chain, and/or changing the carbon skeleton's structure from linear to branched does not change the toxicity profile, or changes the profile in a consistent pattern from lower to higher carbon numbers.

This expectation is supported by a large amount of existing data for alpha and internal olefins with carbon numbers ranging from  $C_6$  to  $C_{54}$ , including data from the OECD SIDS Alpha Olefins Category (1-hexene, 1-decene, 1-dodecene, and 1-tetradecene), which was reviewed and approved at SIAM 11. The data indicate an increasing or decreasing trend or pattern, irrespective of location of double bond or presence or absence of branching, from the shortest olefin in the database ( $C_6$ ) to the longest olefin in the database ( $C_{54}$ ) for various physico-chemical properties and ecotoxicity endpoints (using a mixture of experimental data and estimation techniques), whereas there appears to be no critical difference across category members for biodegradation and health endpoints. Therefore, the category approach is justified, and data for linear and branched alpha and internal olefins were used to characterize the human and environmental health hazards for substances in the Higher Olefins Category.

#### Human Health Hazards

Olefins (alkenes) ranging in carbon number from  $C_6$  to  $C_{24}$  alpha (linear) and internal (linear and branched), and  $C_{24}-C_{54}$  alpha (linear and branched) demonstrate low acute toxicity by the oral, inhalation and dermal routes of exposure: Rat oral  $LD_{50} > 5$  g/kg; rat 4-hr inhalation  $LC_{50}$  range = 110 mg/L (32,000 ppm) to 6.4 mg/L (693 ppm) for  $C_6$  to  $C_{16}$ ; and rat/rabbit dermal  $LD_{50} >$  highest doses tested (1.43-10 g/kg). Repeated dose studies, using the inhalation ( $C_6$  alpha), dermal ( $C_{12}-C_{16}$  alpha), or oral ( $C_6$  alpha and internal linear/branched;  $C_8$  and  $C_{14}$  alpha; and  $C_{16}/C_{18}, C_{18}$  and  $C_{20}-C_{24}$  internal linear/branched) routes of exposure, have shown comparable levels of low toxicity in rats. In females, alterations in body and organ weights, changes in certain clinical chemistry/hematology values, and liver effects were noted (NOELs of  $\geq 100$  mg/kg oral or  $\geq 3.44$  mg/L [1000 ppm] inhalation). In males, alterations in organ weights, changes in certain clinical chemistry/hematology values, liver effects, and kidney damage were noted (LOELs  $\geq 100$  mg/kg oral only). The male rat kidney damage was seen in oral studies with  $C_6, C_8$  and  $C_{14}$

linear alpha olefins and C<sub>6</sub> internal branched olefins, but was not seen in studies with C<sub>16</sub>/C<sub>18</sub> or C<sub>20</sub>-C<sub>24</sub> internal linear/branched olefins. While no specific immunohistochemical staining was conducted to identify the hyaline droplets associated with the observed kidney effects, their morphology and occurrence only in male rats suggest that they are probably related to alpha<sub>2</sub>μ-globulin nephropathy, a male rat specific effect that is not considered relevant to human health. The noted liver effects were seen in oral studies with C<sub>14</sub> alpha olefins (minimal-to-mild hepatocyte cytoplasmic vacuolation with increased liver weight in males and females) and with C<sub>20</sub>-C<sub>24</sub> internal olefins (minimal centrilobular hepatocyte hypertrophy with increased liver weight in females only). No effects were present in the study with C<sub>20</sub>-C<sub>24</sub> internal olefins following a 4-week recovery period, indicating reversibility of the observed effects. These liver effects seen only with the larger molecules may be indirect effects of an intensified liver burden, rather than a direct toxic effect of the olefin. Based on evidence from neurotoxicity screens included in repeated dose studies with C<sub>6</sub> and C<sub>14</sub> alpha olefins and with C<sub>6</sub>, C<sub>16</sub>/C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> internal linear/branched olefins, the category members are not neurotoxic. Based on evidence from reproductive/developmental toxicity screens in rats with C<sub>6</sub> and C<sub>14</sub> alpha olefins and C<sub>6</sub> and C<sub>18</sub> linear/branched internal olefins, along with the findings of no biologically significant effects on male or female reproductive organs in repeated dose toxicity studies, the category members are not expected to cause reproductive or developmental toxicity. Based on the weight of evidence from studies with alpha and internal olefins, category members are not genotoxic. No carcinogenicity tests have been conducted on C<sub>6</sub>-C<sub>54</sub> alpha or internal olefins; however, there are no structural alerts indicating a potential for carcinogenicity in humans. These materials are not eye irritants or skin sensitizers. Prolonged exposure of the skin for many hours may cause skin irritation. The weight of evidence indicates alpha and internal olefins with carbon numbers between C<sub>6</sub> and C<sub>54</sub> have a similar and low level of mammalian toxicity, and the toxicity profile is not affected by changes in the location of the double bond or the addition of branching to the structure. Thus, the data available for the C<sub>6</sub>-C<sub>54</sub> alkenes are adequate to characterize the human health hazards of substances included in the Higher Olefins Category and justify the category designation. The data indicate a low hazard potential for human health for members of the Higher Olefins Category, which is consistent with the conclusion reached at SIAM 11 for the Alpha Olefins Category.

### Hazards to the Environment

The potential for exposure of aquatic organisms to members of the Higher Olefins Category will be influenced by their physico-chemical properties. The predicted or measured water solubilities of these olefins range from 50 mg/L at 20°C for hexene to 0.00015 mg/L at 25°C for 1-octadecene, and to 6.33 [E-23] mg/L at 25°C for C<sub>54</sub> alpha olefin, which suggests there is a lower potential for the larger olefins to be bioavailable to aquatic organisms due to their low solubilities. Their vapor pressures range from 230.6 hPa at 25°C for hexene to 0.00009 hPa at 25°C for 1-octadecene, and to 1.13 [E-16] hPa at 25°C for C<sub>54</sub> alpha olefin, which suggests the shorter chain olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for long periods of time; while the longer chain olefins will tend to partition primarily to water, soil or sediment, depending on water solubility and sorption behavior. The predicted soil adsorption coefficients (K<sub>oc</sub>) range from 149 for C<sub>6</sub> to 230,800 for C<sub>18</sub>, and to 1.0 [E10] for C<sub>54</sub>, indicating increasing partitioning to soil/sediment with increasing carbon number. Level I fugacity modelling predicts that the C<sub>6</sub>-C<sub>13</sub> olefins would partition primarily to air, while the C<sub>16</sub> and longer chain olefins would partition primarily to soil. Results of Level III fugacity modelling suggest that the C<sub>6</sub> - C<sub>8</sub> category members will partition primarily to the water compartment; and, as the chain length increases beyond C<sub>10</sub>, soil and sediment become the primary compartments. These chemicals have a very low potential to

hydrolyze and do not photodegrade directly. However, in the air, all members of the category are subject to atmospheric oxidation from hydroxyl radical attack, with calculated degradation half-lives of 1.8 to 4.8 hours. C<sub>6</sub> – C<sub>30</sub> olefins have been shown to degrade to an extent of approximately 8-92% in standard 28-day biodegradation tests. These results were not clearly correlated with carbon number or any other identifiable parameter; however, the weight of evidence shows that the members of the Higher Olefins Category have potential for degradation in the environment. Volatilization from water is predicted to occur rapidly (hours to days), with Henry's Law Constants (bond method) ranging from 0.423 (C<sub>6</sub>) to 10.7 (C<sub>18</sub>), and to 2.89 [E5] (C<sub>54</sub>) atm·m<sup>3</sup>/mol. Consideration of these degradation processes supports the assessment that these substances will degrade relatively rapidly in the environment and not persist. Based on calculated bioconcentration factors, the C<sub>6</sub>, C<sub>7</sub>, and C<sub>16</sub> and longer chain length category members are not expected to bioaccumulate (BCF: C<sub>6</sub> = 44-46, C<sub>7</sub> = 236, C<sub>16</sub> = 71-92 and ≥ C<sub>18</sub> = 3.2-4.6). Although the C<sub>8</sub> – C<sub>15</sub> olefins have BCFs ranging from 313 to 2030, and K<sub>ow</sub> values ranging from 4.13 to 7.49, and thus are considered to have the potential for bioaccumulation, their physico-chemical properties and fate indicate that there would be limited environmental exposure because of volatility, biodegradability and limited solubility. Data indicate that acute aquatic toxicity can be observed for C<sub>6</sub> through the C<sub>10</sub> olefins (C<sub>6</sub>: EC/LC50 range of 1-10 mg/L; C<sub>7</sub>-C<sub>10</sub>: EC/LC50 range of 0.1-1.0 mg/L), and that toxicity increases with increasing carbon number within that range, which is consistent with increasing K<sub>ow</sub> values (3.07 – 5.12). Above a chain length of 10, toxicity is not observed within the limits of solubility. However, data indicate that chronic aquatic toxicity can be observed in the C<sub>10</sub> olefins (EC10 = 20.0 µg/L, EC50 = 28.1 µg/L, NOEC = 19.04 µg/L). Data also suggest that aquatic toxicity does not differ with bond location or presence of branching. Sufficient data are available to characterize the environmental hazards of members of the Higher Olefins Category.

### Exposure

The following U.S. production volumes for 2002 were reported for members of the Higher Olefins Category: 1-10 million pounds for 8 products, 10-50 million pounds for 5 products, 50-100 million pounds for 9 products, 100-200 million pounds for 5 products, 300-400 million pounds for 1 product, 400-500 million pounds for 1 product, and 700-800 million pounds for 1 product. Members of the Higher Olefins Category are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals (including polymers, fatty acids, mercaptans, plasticizer alcohols, detergents, surfactants, additives for lubricants, amine oxides and amines, detergent alcohols and nonionics, and hydraulic fluids and additives). C<sub>12</sub> to C<sub>20</sub> olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. C<sub>20</sub>-C<sub>54</sub> alpha olefins are used in wax applications. No other non-intermediate applications have been identified. Non-occupational human exposure is limited to exposure to waxes containing C<sub>20</sub>-C<sub>54</sub> alpha olefins. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. Results from modelled data suggest that on-site waste treatment processes are expected to remove these substances from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge. The olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

### RECOMMENDATIONS

The Higher Olefins Category is currently of low priority for further work.

**RATIONALE FOR THE RECOMMENDATION**

The chemicals in this category are currently of low priority for further work. These chemicals possess properties indicating hazards to human health (reversible mild skin and eye irritation; mild respiratory tract irritation to the lower chain length members) and the environment (acute aquatic toxicity for the C<sub>6</sub>-C<sub>10</sub> category members and chronic aquatic toxicity for C<sub>10</sub>). Based on available exposure data for the U.S (five manufacturing sites) and relating to use pattern in the U.S. (primarily as industrial intermediates in closed systems) this category is a low priority for further work.

**AMERICAN CHEMISTRY COUNCIL**

**HIGHER OLEFINS PANEL**

The Higher Olefins Panel includes the following member companies:

BP

Chevron Phillips Chemical Company LP

ExxonMobil Chemical Company

Shell Chemical Company

Shell Chemicals Ltd.

Sasol North America

Spolana a.s. Neratovice

Sunoco, Inc.

## CONTENTS

1	IDENTITY .....	9
1.1	Identification of the Substance .....	9
1.2	Purity/Impurities/Additives .....	10
1.3	Physico-Chemical properties .....	12
1.4	Category Rationale.....	16
2	GENERAL INFORMATION ON EXPOSURE .....	16
2.1	Production Volumes and Use Pattern .....	17
2.2	Environmental Exposure and Fate.....	19
2.2.1	Sources of Environmental Exposure .....	19
2.2.2	Photodegradation.....	19
2.2.2.1	Photodegradation – Direct Photolysis .....	19
2.2.2.2	Photodegradation – Indirect Photolysis (Atmospheric Oxidation).....	19
2.2.3	Stability in Water.....	20
2.2.4	Transport between Environmental Compartments .....	20
2.2.5	Biodegradation .....	22
2.2.6	Bioaccumulation.....	25
2.2.7	Other Information on Environmental Fate .....	25
2.3	Human Exposure .....	25
2.3.1	Occupational Exposure.....	25
2.3.2	Consumer Exposure.....	26
3	HUMAN HEALTH HAZARDS .....	26
3.1	Effects on Human Health.....	26
3.1.1	Toxicokinetics, Metabolism and Distribution .....	26
3.1.2	Acute Toxicity.....	29
3.1.3	Irritation.....	30
3.1.4	Sensitization .....	31
3.1.5	Repeated Dose Toxicity.....	31
3.1.6	Mutagenicity.....	35
3.1.7	Carcinogenicity.....	36
3.1.8	Toxicity for Reproduction .....	36
3.1.9	Neurotoxicity.....	38
3.2	Initial Assessment for Human Health.....	39
4	HAZARDS TO THE ENVIRONMENT .....	39
4.1	Aquatic Effects .....	40
4.2	Terrestrial Effects .....	49
4.3	Other Environmental Effects .....	49
4.4	Initial Assessment for the Environment.....	49
5	RECOMMENDATIONS .....	49

6 REFERENCES.....50

## Tables

Table 1	Identity of members of the Higher Olefins Category.....	9
Table 2	Reported purities/composition/impurities for members of the Higher Olefins Category.....	10
Table 3	Summary of physico-chemical properties for members of the Higher Olefins Category .....	12
Table 4	Reported U.S. production volume for members of the Higher Olefins Category.....	17
Table 5	Typical uses of substances in the Higher Olefins Category.....	18
Table 6	Summary of ready biodegradability tests for members of the Higher Olefins Category .....	24
Table 7	Calculated bioconcentration factors (BCF) for C <sub>6</sub> -C <sub>54</sub> alpha (A) and/or internal (I) olefins .....	25
Table 8	Concentrations of individual 1-alkenes after the third daily 12 hr inhalation exposure to 300 ppm and concentrations in fat 12 hr after the third exposure .....	27
Table 9	Concentrations of individual 1-alkenes after the third daily 12 hr exposure to 100 ppm and after 12 hr recovery .....	27
Table 10	Calculated aquatic toxicity, water solubility and log Kow values for selected C <sub>6</sub> to C <sub>10</sub> internal olefins...	41
Table 11	Calculated aquatic toxicity, water solubility, and log Kow values for selected C <sub>6</sub> to C <sub>10</sub> alpha and internal olefins .....	41
Table 12	Algae toxicity and invertebrate and fish acute toxicity of C <sub>6</sub> -C <sub>24</sub> alkenes.....	42
Table 13	Predicted chronic toxicity results for representative C <sub>6</sub> - C <sub>13</sub> members or components of members of the Higher Olefins Category .....	48
Table 14	Summary of toxicity to microorganisms.....	48
Annex to Category Summary.....		56
Table 1	Environmental fate and transport of the Higher Olefins Category members and selected C <sub>6</sub> -C <sub>54</sub> alpha and internal olefin components of category members. ....	56
Table 2:	Health effects (SIDS endpoints) for Higher Olefins Category members and analogues .....	61
Table 2a:	Irritation and sensitization data for Higher Olefins Category members and analogues/surrogates .....	68
Table 3	Data summary matrix for the Higher Olefins Category members.....	74

## HPV Chemical Category Summary: Higher Olefins Category

### 1 IDENTITY

#### 1.1 Identification of the Substance

The Higher Olefins Category consists of a non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins ( $C_6$  through  $C_{54}$ ) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. All CAS numbers are within the HPV Challenge Program. The  $C_6 - C_{14}$  even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Panel sponsored the  $C_6, C_7, C_8, C_9, C_{10}, C_{12}$  and  $C_{10-13}$  aliphatic predominantly linear internal olefins and the  $C_{16}$  and  $C_{18}$  aliphatic linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). The members of the category are presented in Table 1.

**Table 1** Identity of members of the Higher Olefins Category

Alpha Olefins	Branched/Linear	CAS No.
Neohexene	Branched	558-37-2
1-Tridecene	Linear	2437-56-1
1-Hexadecene (ICCA)	Linear	629-73-2
1-Octadecene (ICCA)	Linear	112-88-9
1-Eicosene	Linear	3452-07-1
1-Docosene	Linear	1599-67-3
1-Tetracosene	Linear	10192-32-2
Alkenes, C10-16 alpha	Linear	68855-58-3
Alkenes, C14-18 alpha	Linear	68855-59-4
Alkenes, C14-20 alpha	Linear	68855-60-7
a-Olefin fraction C20-24 cut	Linear	93924-10-8
a-Olefin fraction C24-28 cut	Branched and Linear	93924-11-9
Alkene, C24-54 branched and linear, alpha	Branched and Linear	131459-42-2
<b>Internal Olefins</b>		
Hexene (ICCA)	Linear	25264-93-1
Heptene (ICCA)	Linear	25339-56-4
Octene (ICCA)	Linear	25377-83-7
Nonene (ICCA)	Linear	27215-95-8
Dodecene (ICCA – not sponsored in HPV)	Linear	25378-22-7
Alkenes, C6	Branched and Linear	68526-52-3
Alkenes, C6-8, C7 rich	Not data available	68526-53-4
Alkenes, C7-9, C8-rich	Linear	68526-54-5
Alkenes, C8-10, C9-rich	Linear	68526-55-6
Alkenes, C9-11, C10-rich	Linear	68526-56-7
Alkenes, C10-12, C11-rich	Linear	68526-57-8
Alkenes, C11-13, C12-rich	Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-10-8
Alkenes, C10-16	Linear	68991-52-6
Alkenes, C15-C18	Linear	93762-80-2
C10,12 Olefin rich hydrocarbons	Linear	68514-32-9

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

C12,14 Olefin rich hydrocarbons	Linear	68514-33-0
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1.2 Purity/Impurities/Additives

The C<sub>6</sub>-C<sub>18</sub> internal olefins included in this category are usually manufactured and marketed as components of linear or linear/branched alkene blends, with small amounts of alpha olefins and/or alkanes of similar chain lengths as impurities. Two category members (C10,12 olefin rich hydrocarbons, CAS No. 68514-32-9; and C12,14 olefin rich hydrocarbons, CAS No. 68514-33-0) contain a significant amount of paraffin. Neohexene is marketed as a pure substance. C<sub>10</sub> – C<sub>18</sub> alpha olefins are manufactured and marketed as blends, but 1-tridecene, 1-hexadecene and 1-octadecene are also sold as relatively pure substances. The C<sub>20</sub> – C<sub>54</sub> alpha olefins are usually manufactured and marketed as alpha olefin blends with small amounts of alpha olefins of higher and lower chain lengths as impurities. The compositions, purities and impurities that have been reported by manufacturers are shown in Table 2.

Table 2 Reported purities/composition/impurities for members of the Higher Olefins Category

Alpha Olefins	CAS No.	Purity	Composition/Impurities
Neohexene	558-37-2	97%	1.5% 2,3-dimethylbutene-1 (CAS No. 563-78-0), branched; related hydrocarbons
1-Tridecene	2437-56-1	100%, 90%	C13 linear. No impurities or branching  Also reported: C12 and lower olefins = 4% max., C13 = 90% min., C14 and higher olefins = 10% max., with max. 8% branched
1-Hexadecene (ICCA)	629-73-2	92%, 80-98%	5.5-6.8% vinylidenes (branching at 2 <sup>nd</sup> carbon), max. 7% C14 and lower olefins, max. 15% C18 and higher olefins
1-Octadecene (ICCA)	112-88-9	90.6%, >91% and 80-98%	7.7% vinylidenes (branching at 2 <sup>nd</sup> carbon), max. 5% C16 and lower olefins, max. 20% C20 and higher olefins
1-Eicosene	3452-07-1	100%	C20 linear. No impurities or branching
1-Docosene	1599-67-3	100%	C22 linear. No impurities or branching
1-Tetracosene	10192-32-2	100%	C24 linear. No impurities or branching
Alkenes, C10-16 alpha	68855-58-3	NA	Typical composition: 0.6% C10, 64.2% C12, 34.7% C14, 0.5% C16; 99.6% monoolefin; 0.4% paraffin; 86.5% linear terminal; 10.6% branched terminal; 2.9% linear internal
Alkenes, C14-18 alpha	68855-59-4	NA	Typical composition: 1% C12, 65% C14, 33% C16, 1% C18; 99.5% monoolefin; 0.5% paraffin; 82.0% linear terminal; 14% branched terminal; 4% linear internal
Alkenes, C14-20 alpha	68855-60-7	NA	Typical composition: 1% C14, 57% C16, 37% C18, 5% C20; 99.2% monoolefin; 0.8% paraffin; 61.5% linear terminal; 32.5% branched terminal; 6% linear internal

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

a-Olefin fraction C20-24 cut	93924-10-8	NA	Max. composition: 3% C18, 47% C20, 35% C22, 26% C24, 1% C26, 89.3% linear, 8.3% branched, 0.3% paraffin.  Also reported: C18 = max.5%, C20 = 45-60%, C22 = 30-50%, C24 = max.15%, C26 = max.1%
a-Olefin fraction C24-28 cut	93924-11-9	NA	Max. composition: 9% C24, 18% C26, 17% C28, 12% C30, 0.8% paraffin, 0.6% paraffin
Alkene, C24-54 branched and linear, alpha	131459-42-2	NA	Max. 28% C28 and lower carbon number, min. 72% C30+, 33-39% branched, >50% linear alpha olefin, 10% internal olefins
<b>Internal Olefins</b>			
Hexene (ICCA)	25264-93-1	NA	C6-C8 internal olefin blend: Typical composition = 1.9% C <sub>5</sub> , 43.3% C <sub>6</sub> , 21.7% C <sub>7</sub> , 31.7% C <sub>8</sub> , 1.4% C <sub>9</sub>
Heptene (ICCA)	25339-56-4	NA	C6-C8 internal olefin blend: Typical composition = 1.9% C <sub>5</sub> , 43.3% C <sub>6</sub> , 21.7% C <sub>7</sub> , 31.7% C <sub>8</sub> , 1.4% C <sub>9</sub>
Octene (ICCA)	25377-83-7	NA	C6-C8 internal olefin blend: Typical composition = 1.9% C <sub>5</sub> , 43.3% C <sub>6</sub> , 21.7% C <sub>7</sub> , 31.7% C <sub>8</sub> , 1.4% C <sub>9</sub>
Nonene (ICCA)	27215-95-8	Nda	Nda
Dodecene (ICCA – not sponsored in HPV)	25378-22-7	NA	C10-13 internal olefin blend: Typical composition = <0.1% C <sub>9</sub> or lower, 11.2% C <sub>10</sub> , 29.6% C <sub>11</sub> , 25.9% C <sub>12</sub> , 23.6% C <sub>13</sub> , 9.5% C <sub>14</sub> and 0.1 % >C <sub>14</sub> ; with 4.2% N-paraffins and 4.6% dienes as impurities
Alkenes, C6	68526-52-3	NA	Typical composition: 0.5% C <sub>5</sub> n-olefins, 1.3% C <sub>5</sub> iso-olefins, 10.4% C <sub>6</sub> n-olefins, 55.6% C <sub>6</sub> iso-olefins, 3.3% C <sub>5</sub> n-paraffins, 9.3% C <sub>5</sub> iso-paraffins, 17.8% C <sub>6</sub> iso-paraffins, 1.0% C <sub>7</sub> iso-olefins
Alkenes, C6-8, C7 rich	68526-53-4	NA	Typical composition: 1% C <sub>6</sub> olefins, 97% C <sub>7</sub> olefins, 2% C <sub>8</sub> olefins.
Alkenes, C7-9, C8-rich	68526-54-5	NA	Mostly linear, less than 5% branched. Typical composition: 1% C <sub>7</sub> olefins, 89% C <sub>8</sub> olefins, 10% C <sub>9</sub> olefins.
Alkenes, C8-10, C9-rich	68526-55-6	NA	Mostly linear, less than 2% branched. Typical composition: 1% C <sub>8</sub> olefins, 91% C <sub>9</sub> olefins, 8% C <sub>10</sub> olefins.
Alkenes, C9-11, C10-rich	68526-56-7	NA	Mostly linear, less than 2% branched. Typical composition: 5% C <sub>9</sub> olefins, 84% C <sub>10</sub> olefins, 10% C <sub>11</sub> olefins, 0.2% C <sub>12</sub> olefins; or  Max. 5% C <sub>9</sub> and lower, minimum 94% C <sub>10</sub> , max. 3% C <sub>11</sub> and higher, with max. 10% branched
Alkenes, C10-12, C11-rich	68526-57-8	NA	Typical composition: 1% C <sub>9</sub> olefins, 10% C <sub>10</sub> olefins, 76% C <sub>11</sub> olefins, 13% C <sub>12</sub> olefins.  Also reported: Mostly linear, less than 2% branched.
Alkenes, C11-13, C12-rich	68526-58-9	NA	Mostly linear, less than 2% branched.
Heavy polymerization naphtha (petroleum)	68783-10-8	NA	Branched, C11-13, C12-rich olefins

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Alkenes, C10-16	68991-52-6	NA	Mostly linear, less than 2% branched.
Alkenes, C15-C18	93762-80-2	NA	Mostly linear, less than 2% branched.
C10,12 Olefin rich hydrocarbons	68514-32-9	NA	0-1% C8, 10-30% C10, 70-90% C12, 0-1% C14, 0-50% paraffins
C12,14 Olefin rich hydrocarbons	68514-33-0	NA	0-8% C12 and lower, 92-100% C14, 0-0.2% C16, 0-1% C14, 0-50% paraffins

NA: Not applicable – Substance is manufactured and marketed as a component of a blend, or is a blend with variable composition.

Nda: No data available

1.3 Physico-Chemical properties

Table 3 Summary of physico-chemical properties for members of the Higher Olefins Category and for representative components of category members<sup>a</sup>

Chemical Name [Category members are in bold type]	Melting Point (°C)	Boiling Point (°C)	Vapour Pressure	Density/ Relative Density	Partition Coefficient (Log K <sub>ow</sub> )	Water Solubility (mg/L)
<b>Hexene (CAS No. 25264-93-1)</b>	-98 (m)	65 [hexene - mix of isomers] at 1013 hPa (m)  66.4 – 68.8 [2-hexene, 3-hexene] (m)	230.6 hPa at 25°C ) (m and c)	0.68-0.69 g/cm <sup>3</sup> at 20°C [2-hexene]	3.07 (c)  3.39 at 25°C [1-hexene] (m)	50 at 20°C (m)
<b>Neo-Hexene (CAS No. 558-37-2)</b>	-115.2(m)	41.2 at 1013 hPa (m)	574.6 hPa at 25°C (m)	0.66 at 15.6/15.6°C (relative density)	3.04 (c)	32.53 at 25°C (c)
<b>Alkenes, C6 (CAS No. 68526-52-3)</b>	-95.3 (c)	69.66 at 1013 hPa (c)	245.0 hPa at 25°C (c)	nda	3.15 at 25°C (c)	47.5 at 25°C (c)
<b>Heptene (CAS No. 25339-56-4)</b>	-82.4 (c)  -119.7 [1-heptene] (m)	94.35 at 1013 hPa (c)  93.6 at 1013 hPa [1-heptene] (m)	74.66 hPa at 25°C (c)  79.05 hPa at 25°C [1-heptene] (m)	ca. 700 k g/m <sup>3</sup> at 20°C [C <sub>6</sub> -C <sub>8</sub> internal olefin]	3.64 (c)  3.99 [1-heptene] (m)	13.45 at 25°C (c)  18.2 at 25°C [1-heptene] (m)
<b>Alkenes, C6-8, C7-rich (CAS No. 68526-53-4)</b>	-82.4 (c)	94.35 at 1013 hPa (c)	74.66 hPa at 25°C (c)	nda	3.64 at 25 °C (c)	13.45 at 25°C (c)

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

<b>Chemical Name</b> [Category members are in bold type]	<b>Melting Point (°C)</b>	<b>Boiling Point (°C)</b>	<b>Vapour Pressure</b>	<b>Density/ Relative Density</b>	<b>Partition Coefficient (Log K<sub>ow</sub>)</b>	<b>Water Solubility (mg/L)</b>
<b>Octene (CAS No. 25377-83-7)</b>	-109 (m)  < -74 (m)	123 at 1013 hPa (m)	22 hPa at 25°C (c)  23.2 hPa at 25°C [1-octene] (m)	0.72 g/cm <sup>3</sup> at 20°C  [2-octene]	4.13 (c)  4.57 [1-octene] (m)	3.65 at 25°C(c)  4.1 at 25°C [1-octene] (m)
<b>Alkenes C7-9, C8-rich (CAS No. 68526-54-5)</b>	-69.84 (c)	118.13 at 1013 hPa (c)  110 – 126 (m)	22 hPa at 25°C (c)	0.73 g/cm <sup>3</sup> at 20°C (m)	4.13 (c)	3.89 at 25°C (c)
<b>Nonene (CAS No. 27215-95-8)</b>	-56.70 (c)  -81.3 [1-nonene] (m)	149.53 at 1013 hPa (c)  135 – 140 at 1013 hPa (m)	5.00 hPa at 25°C (m)	0.74 g/cm <sup>3</sup> at 20°C	4.55 (c)	3.619 at 25°C (c)
<b>Alkenes, C8-10, C9-rich (CAS No. 68526-55-6)</b>	-57.53(c)	141.02 at 1013 hPa (c)  146.9 at 1013 hPa [isononene] (m)	7.85 hPa at 25°C (c)  7.2 hPa at 25°C [isononene] (m)	0.75 g/cm <sup>3</sup> at 15°C (m)	4.62 (c)  5.15 at 25 °C [isononene] (m)	1.104 at 25°C (c)  1.12 at 25°C [isononene] (m)
<b>Decene (CAS No. 25339-53-1)</b>	-45.48 (c)	170 at 1013 hPa (m)	1.33 hPa at 14.7°C (m)  2.79 hPa at 25°C (c)	0.74 g/cm <sup>3</sup> at 20°C	5.12 (c)	0.3288 at 25°C (c)
<b>1-Decene (CAS No. 872-05-9)</b>	-66.3 (m)	170.5 at 1013 hPa (m)	2.23 hPa at 25°C (m)	nda	5.7 (m)	0.57 at 25°C (m)  0.210 at 25°C (m)
<b>Alkenes, C9-11, C10-rich (CAS No. 68526-56-7)</b>	-46.7 (c)	176.1 at 1013 hPa (c)	2.1 hPa at 25°C (c)	nda	4.69 (c)	2.51 at 25°C (c)
<b>C10,12 Olefin rich hydrocarbons (CAS No. 68514-32-9)</b>	-48.7 (c)	181 at 1013 hPa (c)	1.69 hPa at 25°C (c)	nda	4.33 (c)	5.2 at 25°C (c)
<b>Alkenes, C10-12, C11-rich (CAS No. 68526-57-8)</b>	-33.69 (c)	184.07 at 1013 hPa (c)	0.975 hPa at 25°C (c)	nda	5.61 at 25 °C (c)	0.3432 at 25°C (c)

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical Name [Category members are in bold type]	Melting Point (°C)	Boiling Point (°C)	Vapour Pressure	Density/ Relative Density	Partition Coefficient (Log K <sub>ow</sub> )	Water Solubility (mg/L)
Undecene (CAS No. 28761-27-5, mix of isomers)	-77 (m)	194 at 1013 hPa (m)	0.917 hPa at 25°C (c)  0.66 hPa at 25°C (m)	nda	5.53 (c)	0.4006 at 25°C (c)
<b>Dodecene (CAS No. 25378-22-7)</b>	-35.2 (m)	213.8 at 1013 hPa (m)	0.356 hPa at 25°C (c)	0.77 at 20°C (relative density)	6.10 (c)	0.1245 at 25°C (c) 0.131 [2-dodecene] (c)
1-Dodecene (CAS No. 112-41-4)	-35.2 (m)	213.8 at 1013 hPa (m)	0.212 hPa at 25°C (m)	0.76 g/cm <sup>3</sup>	6.10 (c)	0.113 (c)
<b>Alkenes, C11-13, C12-rich (CAS No. 68526-58-9)</b>	-22.2 (c)	204.24 at 1013 hPa (c)	0.356 hPa at 25°C (c)	0.77 g/cm <sup>3</sup> at 15°C (m)	6.10 at 25°C (c)	0.1127 at 25°C (c)
<b>Heavy polymerization naphtha (petroleum) (CAS No. 68783-10-8) (C11-13, C12 rich alkenes)</b>	nda	nda	nda	nda	nda	nda
<b>C12,14 Olefin rich hydrocarbons (CAS No. 68514-33-0)</b>	-24.2 (c)	229.23 at 1013 hPa (c)	0.167 hPa at 25°C (c)	nda	5.37 (c)	0.4989 at 25°C (c)
<b>1-Tridecene (CAS No. 2437-56-1)</b>	-13 (m)	233 at 1013 hPa (m)	0.085 hPa at 25°C (m)	0.77 (m) (relative density)	6.59 (c)	0.0367 at 25°C (c)
Tridecene (CAS No. 25377-82-6)	-10.9 (c)	224 at 1013 hPa (c)	0.140 hPa at 25°C (c)	nda	6.59 (c)	0.0367 at 25°C (c)
1-Tetradecene (CAS No. 1120-36-1)	-12 (m)	252.10 at 1013 hPa (m)	0.012 hPa at 25°C (m)	0.77 g/cm <sup>3</sup> at 20 °C (m)	7.08 (c)	0.0135 at 25°C (c)
Tetradecene (CAS No. 26952-13-6)	0.41 (c)	248.65 at 1013 hPa (c)	0.063 hPa at 25°C (c)	nda	7.00 (c)	0.0139 at 25°C (c)
Pentadecene (CAS No. 27251-68-9)	11.04 (c)	265.77 at 1013 hPa (c)	0.0261 hPa at 25°C (c)	nda	7.49 (c)	0.0045 at 25°C (c)
<b>1-Hexadecene (CAS No. 629-73-2)</b>	4.1 (m)	284.9 at 1013 hPa (m)	0.0035 hPa at 25°C (m)	0.79 at 15.6/15.6°C (relative density)	8.06 (c)	0.0014 at 25°C (c)
Hexadecene	0.21 (c)	281.97 at 1013 hPa (c)	0.0118 hPa at 25°C (c)	nda	7.98 (c)	0.0014 at 25°C (c)

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical Name [Category members are in bold type]	Melting Point (°C)	Boiling Point (°C)	Vapour Pressure	Density/ Relative Density	Partition Coefficient (Log K <sub>ow</sub> )	Water Solubility (mg/L)
<b>1-Octadecene</b> (CAS No. 112-88-9)	18.3 (m)	315 at 1013 hPa (m)	0.00009 hPa at 25°C (m) 0.00085 – 0.0013 hPa at 25 (c) <sup>b</sup>	0.79 at 15.6/15.6°C (relative density)	>8 (m )  9.04 (c)	0.0001508 at 25°C (c )
Octadecene (CAS No. 27070-58-2)	29.6 (m)	306.27 at 1013 hPa (c)	0.0035 hPa at 25 (c)	nda	9.04 (c)	0.0001256 at 25°C (c )
<b>Alkenes, C10-16 alpha</b> (CAS No. 68855-58-3)	nda	nda	nda	nda	nda	nda
<b>Alkenes C10-16</b> (CAS No. 68991-52- 6)	nda	nda	nda	nda	nda	nda
<b>Alkenes C14-18 alpha</b> (CAS No. 68855-59-4)	nda	nda	nda	nda	nda	nda
<b>Alkenes C14-20 alpha</b> (CAS No. 68855-60-7)	nda	nda	nda	nda	nda	nda
<b>Alkenes C15-C18</b> (CAS No. 93762-80- 2)	nda	nda	nda	nda	nda	nda
<b>1-Eicosene</b> (CAS No. 3452-07-1)	28.5 (m)	341 at 1013 hPa (m)	0.0000141 hPa at 25°C (e)  0.0005453 hPa (c)	0.79 at 30°C (c) (relative density)	10.03 (c)	1.264 [E-5] at 25°C (c)
<b>1-Docosene</b> (CAS No. 1599-67-3)	38 (m)	367 at 1013 hPa (m)	0.000115 hPa at 25°C (c)	0.79 at 30°C (c) (relative density)	11.01 (c)	1.259 [E-6] at 25°C (c)
<b>1-Tetracosene</b> (CAS No. 10192-32-2)	96.76 (c)	379.97 at 1013 hPa (c)	0.0000153 hPa at 25°C (c)	0.79 at 30°C (c) (relative density)	11.99 (c)	1.244 [E-7] at 25°C (c)
<b>1-Hexacosene</b> (CAS No. 18835-33-1)	114.81 (c)	403.17 at 1013 hPa (c)	0.00000288 hPa at 25°C (c)	nda	12.97 (c)	1.22 [E-8] at 25°C (c)
<b>1-Octacosene</b> (CAS No. 18835-34-2)	132.85 (c)	426.38 at 1013 hPa (c)	0.00000053 hPa at 25°C (c)	nda	13.96 (c)	1.19[E-9] at 25°C (c)
<b>1-Triacontene</b> (CAS No. 18435-53-5)	150.90 (c)	449.59 at 1013 hPa (c)	9.4 [E-8] hPa at 25°C (c)	nda	14.94 (c)	1.155[E-10] at 25°C (c)

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

<b>Chemical Name</b> [Category members are in bold type]	<b>Melting Point (°C)</b>	<b>Boiling Point (°C)</b>	<b>Vapour Pressure</b>	<b>Density/ Relative Density</b>	<b>Partition Coefficient (Log K<sub>ow</sub>)</b>	<b>Water Solubility (mg/L)</b>
C54 alpha Olefin	319.14 (c)	728.08 at 1013 hPa (c)	1.13 [E-16] hPa at 25°C (c)	nda	26.72 (c)	6.33 [E-23] at 25°C (c)
<b>a-Olefin fraction C20-24 cut (CAS No. 93924-10-8)</b>	nda	nda	nda	nda	nda	nda
<b>a-Olefin fraction C24-28 cut (CAS No. 93924-11-9)</b>	nda	nda	nda	nda	nda	nda
<b>Alkene, C24-54 branched and linear, alpha (CAS No. 131459-42-2)</b>	nda	nda	nda	nda	nda	nda

<sup>a</sup> Calculated (c), Measured (m), Extrapolated from measured data (e), No data available (nda)

<sup>b</sup> NOMOS estimate using two measured values at higher temperature and reduced boiling points

The C<sub>6</sub>-C<sub>16</sub> members of the category are colorless liquids; C<sub>18</sub> is a colorless liquid or white solid depending on ambient temperature; and C<sub>20</sub>-C<sub>54</sub> members are white solids. Vapor pressure and water solubility decrease with increasing chain length, while melting point, boiling point, and octanol:water partition coefficients increase with increasing chain length. The characteristic feature of the alkene structure is the C=C double bond. The characteristic reactions of an alkene are those that take place at the double bond, the most typical being an electrophilic addition reaction.

#### 1.4 Category Rationale

Due to similarities of this non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins (C<sub>6</sub> through C<sub>54</sub>) under 30 CAS numbers (13 for alpha olefins and 17 for internal olefins), a category approach was utilized. All CAS numbers are within the EPA's HPV Chemical Challenge Program. The C<sub>6</sub> - C<sub>14</sub> even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Higher Olefins Panel sponsored the C<sub>6</sub>, C<sub>7</sub>, C<sub>8</sub>, C<sub>9</sub>, C<sub>10</sub>, C<sub>12</sub> and C<sub>10-13</sub> predominantly linear internal olefins and the C<sub>16</sub> and C<sub>18</sub> linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). For the purposes of the EPA HPV Chemical Challenge Program, the category was defined as "Higher Olefins." The category designation was based on the belief that internalizing the location of the carbon-carbon double bond, increasing the length of the carbon chain, and/or changing the carbon skeleton's structure from linear to branched does not change the toxicity profile, or changes the profile in a consistent pattern from lower to higher carbon numbers.

This expectation is supported by a large amount of existing data for alpha and internal olefins with carbon numbers ranging from C<sub>6</sub> to C<sub>54</sub>, including data from the OECD SIDS Alpha Olefins Category (1-hexene, 1-decene, 1-dodecene, and 1-tetradecene), which was reviewed and approved at SIAM 11. The data indicate an increasing or decreasing trend or pattern, irrespective of location of double bond or presence or absence of branching, from the shortest olefin in the database (C<sub>6</sub>) to the longest olefin in the database (C<sub>54</sub>) for various physico-chemical properties and ecotoxicity endpoints (using a mixture of experimental data and estimation techniques), whereas there appears to be no critical difference across category members for biodegradation and health endpoints. Therefore, the category approach is justified, and data for linear and branched alpha and internal

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

olefins were used to characterize the human and environmental health hazards for substances in the Higher Olefins Category. The data summary matrix for members of the Higher Olefins Category is presented in the Annex, Table 3.

### 2 GENERAL INFORMATION ON EXPOSURE

This section provides available information on substances within the Higher Olefins Category regarding production volume and use, environmental exposure and fate, and human exposure.

#### 2.1 Production Volumes and Use Pattern

In 1999, linear alpha olefins (C<sub>4</sub>-C<sub>30</sub>) global production was approximately 4.9 billion pounds (2.2 million metric tons) with the United States accounting for almost 64% (SRI, 2000). In 2000, global production of nonene was approximately 1,037 million pounds (470,000 metric tons) with the United States accounting for almost 56%; and global production for dodecene was approximately 695 million pounds (315,000 metric tons) with the United States accounting for 47% (SRI, 2001). There are five manufacturing sites in the United States that produce at least one of the members of this category.

Table 4 below, provides a range of U.S. production volumes by substance, provided by the members of the American Chemistry Council's Higher Olefins Panel.

**Table 4** Reported U.S. production volume for members of the Higher Olefins Category

COMPOUND	CAS NUMBER	2002 PRODUCTION VOLUME * (Million Pounds)
<b>Alpha Olefins</b>		
Neohexene	558-37-2	1-10
1-Tridecene	2437-56-1	1-10
1-Hexadecene (ICCA)	629-73-2	100-200
1-Octadecene (ICCA)	112-88-9	100-200
1-Eicosene	3452-07-1	50-100
1-Docosene	1599-67-3	50-100
1-Tetracosene	10192-32-2	10-50
Alkenes, C10-16 alpha	68855-58-3	1-10
Alkenes, C14-18 alpha	68855-59-4	1-10
Alkenes, C14-20 alpha	68855-60-7	50-100
a-Olefin fraction C20-24 cut	93924-10-8	50-100
a-Olefin fraction C24-28 cut	93924-11-9	100-200
Alkene, C24-54 branched and linear, alpha	131459-42-2	50-100
<b>Internal Olefins</b>		
Hexene (ICCA)	25264-93-1	1-10
Heptene (ICCA)	25339-56-4	50-100
Octene (ICCA)	25377-83-7	50-100

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

COMPOUND	CAS NUMBER	2002 PRODUCTION VOLUME <sup>a</sup> (Million Pounds)
Nonene (ICCA)	27215-95-8	100-200
Dodecene (ICCA – not sponsored in HPV)	25378-22-7	1-10
Alkenes, C6	68526-52-3	10-50
Alkenes, C6-8, C7 rich	68526-53-4	10-50
Alkenes, C7-9, C8-rich	68526-54-5	10-50
Alkenes, C8-10, C9-rich	68526-55-6	300-400
Alkenes, C9-11, C10-rich	68526-56-7	50-100
Alkenes, C10-12, C11-rich	68526-57-8	50-100
Alkenes, C11-13, C12-rich	68526-58-9	100-200
Heavy polymerization naphtha (petroleum)	68783-10-8	50-100
Alkenes, C10-16	68991-52-6	400-500
Alkenes, C15-C18	93762-80-2	700-800
C10,12 Olefin rich hydrocarbons	68514-32-9	1-10
C12,14 Olefin rich hydrocarbons	68514-33-0	1-10

<sup>a</sup> Range of production volume submitted by Higher Olefin Panel members to Panel Manager.

There are three main ethylene oligomerization processes currently in use. One process uses a single stage for chain growth and displacement reactions, another uses two separate steps for chain growth and displacement and a third uses a more complex process involving isomerization-disproportionation. Members of the Higher Olefins Category are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals (including polymers, fatty acids, mercaptans, plasticizer alcohols, surfactants, additives for lubricants, amine oxides and amines, detergent alcohols and nonionics, and hydraulic fluids and additives). C<sub>12</sub> – C<sub>20</sub> olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. C<sub>20</sub> – C<sub>54</sub> alpha olefins are used in wax applications. No other non-intermediate applications have been identified. Table 5 provides typical uses by chain length (SRI, 2000; American Chemistry Council, Higher Olefins Panel, 2002).

**Table 5 Typical uses of substances in the Higher Olefins Category**

CHAIN LENGTH	APPLICATION
C <sub>4</sub> -C <sub>8</sub>	Intermediates in the production of polymers and polyethylene
C <sub>6</sub> -C <sub>8</sub>	Intermediates in the production of low-molecular weight fatty acids and mercaptans
C <sub>6</sub> -C <sub>10</sub>	Intermediates in the production of plasticizer alcohols and surfactants
C <sub>10</sub> -C <sub>12</sub>	Intermediates in the production of polyalphaolefins and other additives for lubricants, detergent alcohols; amine oxides and amines
C <sub>10</sub> -C <sub>16</sub>	Intermediates in the production of detergent alcohols and nonionics

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

C <sub>12</sub> -C <sub>20</sub>	Direct components of drilling fluids for off-shore oil exploration
C <sub>16</sub> -C <sub>18</sub>	Intermediates in the production of lube oil additives, surfactants, hydraulic fluids and additives and used as direct components of drilling fluids for off-shore oil extrapolation
C <sub>20</sub> -C <sub>24</sub>	Wax applications [e.g., candles, board/box coatings, polishes]; intermediates for lube oil additives, epoxides used for epoxy resins and polyurethanes, chlorinated plasticizers for PVC, fire retardant agents, additives for metal working fluids
C <sub>24</sub> -C <sub>28</sub>	Wax applications [e.g., candles, board/box coatings, polishes]; intermediates for lube oil additives, epoxides used for epoxy resins and polyurethanes, additives for metal working fluids
C <sub>24</sub> -C <sub>54</sub>	Wax applications [e.g., candles, board/box coatings, polishes]; intermediates for lube oil additives, additives for metal working fluids, lubricants for PVC extrusion

## 2.2 Environmental Exposure and Fate

### 2.2.1 Sources of Environmental Exposure

The members of the Higher Olefins Category are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals (including polymers). C<sub>16</sub> and C<sub>18</sub> olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. C<sub>20</sub> – C<sub>54</sub> alpha olefins are used in wax applications. Results from modelled data suggest that on-site waste treatment processes are expected to remove these compounds from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge (EPIWIN, 2000b). None of the compounds within the category are on the US Toxic Release Inventory (TRI) list (NLM, 2003a). The olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

### 2.2.2 Photodegradation

#### 2.2.2.1 Photodegradation – Direct Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Light at wavelengths longer than 750 nm does not contain sufficient energy to break chemical bonds. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Olefins with one double bond, such as members of this category, do not absorb appreciable light energy above 290 nm (Harris, 1982a). Thus, direct photolysis will not significantly contribute to the degradation of chemicals in the Higher Olefins Category.

#### 2.2.2.2 Photodegradation – Indirect Photolysis (Atmospheric Oxidation)

Indirect photodegradation can be measured (US EPA, 1999a; OECD test guideline 113) or estimated using models (US EPA, 1999b). An estimation method includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation is a result of hydroxyl radical attack and is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Hydrocarbons, such as the majority of the chemicals in this

category, readily volatilize to air. In air, chemicals may undergo reaction with photosensitized oxygen in the form of ozone and hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 2000a, b) calculates a chemical half-life based on an overall hydroxyl radical (OH) reaction rate constant, a 12-hr day, and a given OH concentration (average global concentration of  $1.5 \times 10^6$  OH/cm<sup>3</sup>). It also estimates the rate constant for the gas-phase reaction between ozone and olefinic compounds. Estimated photodegradation hydroxyl radical and ozone reaction rate constants for the substances in the category are in close agreement across the category. In the air, all members of the category are subject to atmospheric oxidation from hydroxyl radical attack, with calculated degradation half-lives of 1.6 to 4.8 hours (see Annex, Table 1), which suggests that, once volatilized to the air, these chemicals will degrade rapidly.

### 2.2.3 Stability in Water

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H<sub>2</sub>O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (Harris, 1982b) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions, the carbon-carbon double bond found in alkenes, such as those in the Higher Olefins Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

The substances in the Higher Olefins Category are primarily olefins that contain one double bond (alkenes). Saturated hydrocarbons (alkanes) are found in category members, generally as impurities. These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Higher Olefins Category have a very low potential to hydrolyse, and this degradative process will not contribute to their removal in the environment.

### 2.2.4 Transport between Environmental Compartments

The vapour pressures of the members of the Higher Olefins Category range from 230.6 hPa at 25°C for hexene to 0.00009 hPa at 25°C for 1-octadecene, and to 1.13 [E-16] hPa at 25°C for C<sub>54</sub> alpha olefin, which suggests the shorter chain olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for long periods of time; while the longer chain olefins will tend to partition primarily to water, soil or sediment, depending on water solubility and sorption behavior. Volatilization from water is predicted to occur rapidly (hours to days), with Henry's Law Constants (bond method) ranging from 0.423 (C<sub>6</sub>) to 10.7 (C<sub>18</sub>), and to 2.89[E5] (C<sub>54</sub>) atm m<sup>3</sup>/mol. The soil adsorption coefficients (K<sub>oc</sub>) range from 149 for C<sub>6</sub> to 230,800

for  $C_{18}$ , to 1.0[E10] for  $C_{54}$ , indicating increasing partitioning to soil/sediment with increasing carbon number.

Fugacity based multimedia modelling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). Widely used fugacity models are the EQC (Equilibrium Criterion) Level I model (Mackay et al., 1996b; Trent University, 2004; EPIWIN, 2000b) and the Mackay Level III fugacity model (Mackay, 1991; Mackay et al., 1996a, 1996b; Trent University, 2004; EPIWIN, 2000b).

The input data required to run a Level I model include basic physico-chemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition. The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapour pressure, and water solubility to calculate distribution within a standardized regional environment. This model (Trent University, 2004) was used, with input values taken from Table 3, to calculate distribution values for selected substances in the Higher Olefins Category. Results from Level I modelling are shown in Annex, Table 1. Level I modelling predicts that the  $C_6$ - $C_{13}$  olefins would partition primarily to air, while the  $C_{16}$ - $C_{54}$  olefins would partition primarily to soil.

A Level III fugacity model (Trent University, 2004) was also used to calculate distribution values for selected members or surrogates of members of the Higher Olefins Category. For olefins with  $\geq 26$  carbon atoms, the EPIWIN Level III Model (EPIWIN, 2000b) was used, as the Trent model did not appear to be suitable for these substances. A Level III fugacity model calculates the distribution of a chemical under steady state, non-equilibrium conditions; and can show the percent distribution and estimates of chemical concentrations in each of the six environmental compartments cited in the Level I discussion above. In comparison to a Level I model, the Level III calculations consider degradation, advection, and intermedia transport processes. Results of the Level III fugacity analysis are sensitive to the relative amounts of the emissions data used in the model calculations. Emissions rate data are needed for the air, water and soil compartments. If emissions data are not available for a chemical, the model uses default emissions, which are 1000 kg/hr each into air, water, and soil; and 0 kg/hr into sediment. These default values and physico-chemical property values from Table 3 were used in the model calculations for the members of the Higher Olefins Category. Percent distribution results for the Higher Olefins category are presented in the Annex, Table 1.

Results of the Level III modelling for members/surrogates of the Higher Olefins Category suggest that the water compartment is the primary environmental compartment to which  $C_6$ - $C_8$  olefins will partition. As the chain length increases beyond  $C_{10}$ , soil and sediment become the primary compartments, followed by water and then air. The prediction that the higher molecular weight olefins will partition to soil/sediment is a consequence of their high organic/carbon partition coefficients ( $K_{oc}$ ) (see Annex, Table 1). This can be attributed to the olefins having a high tendency to bind to particulate matter in the water column, thus binding more to soil and sediment. The larger the olefins are in chain length, the less persistent they are in the atmosphere and water. However, in soil and sediment the olefins increase in persistence with increasing chain length. As biodegradation results (Table 6) indicate that there is no real trend of decreasing biodegradation as the chain length increases, the decreased percentages found in the solid phases are likely due more to increasing sorption and reduced leaching and volatilization.

The fact that results of Level I and Level III fugacity models differ is not unexpected because of the different assumptions made in the models. Level I models evaluate the relative environmental distribution at equilibrium or steady state. Level III models reflect equilibrium partitioning but also the loading factors, modelled as continuous releases to all media. The Level III model used default values for releases that are relatively large. Consequently, the quantities in the Model III compartments do not reflect equilibrium conditions as much as the continuous input values.

Swann et al. (1983) reported that a chemical with a  $K_{oc}$  value between 150 and 500 would move through the soil at a moderate rate. This rate slows between 500 and 2,000. Chemicals with  $K_{oc}$  values between 2,000 and 5,000 can be considered to have practically no mobility, and may be considered immobile at values greater than 5,000. The estimated (EPIWIN, 2000b)  $K_{oc}$  data (Annex, Table 1) show that the lower chain olefins have  $K_{oc}$  values (149, 275, 507 for  $C_6$ ,  $C_7$  and  $C_8$ , respectively) which indicate a potential to migrate through a soil horizon to ground water at a moderate rate. As the carbon number increases, the potential for these chemicals to migrate through soil decreases to the degree that  $C_{12}$  and higher carbon number olefins ( $K_{oc}$  values  $\geq 5864$ ) have only a negligible, if any, potential for migration. These are general characterizations based on the  $K_{oc}$  values for these chemicals, which with increasing carbon number show that there is an increasing tendency to sorb to organic matter. As the sorptive potential increases for a chemical, it will tend to remain bound to organic matter rather than dissolve into water and migrate with the percolating water.

Actual migration through a soil horizon will be influenced by several physical characteristics of the environment and chemical. One chemical characteristic that can significantly impact the relative amounts of these chemicals that will remain available to migrate through soil is volatility. The  $C_6$ - $C_{10}$  olefins have a vapor pressure of greater than 1 mm Hg (1.33 hPa), suggesting that they will tend to volatilize from surface soils at a relatively rapid rate. In comparison, the  $C_{12}$  and higher olefins have vapor pressures less than 1 mm Hg, suggesting that volatilization will have a lesser impact on their loss from surface soils. As a result, the loss of the higher chain olefins from surface soils may be influenced more by biodegradation because they have a lower potential to migrate and volatilize.

### 2.2.5 Biodegradation

Existing data for selected chemicals in the Higher Olefins Category and structural analogs of  $C_6$ - $C_{30}$  category members show that chemicals in the Higher Olefins Category can biodegrade aerobically to a large extent within a few weeks (Table 6).  $C_6$ - $C_{30}$  olefins have been shown to degrade to an extent of approximately 8 to 92% in standard 28-day biodegradation tests. Although no experimental results are available for some category members, results for studies with surrogate or component chemicals suggest that the category members would achieve degradation rates in the general range of 20-70% within 28 days in a standard biodegradation test.

While, in total, biodegradation tests indicate the category is biodegradable and thus non persistent, the data vary over a wide range. Both structural features and test conditions can have an effect on biodegradation results. Carbon number, location of the double bond (internal vs. alpha) and branching are structural features that can affect biodegradability. Inoculum source and concentration, substrate concentration, and use of dispersants to enhance solubility of poorly soluble compounds are examples of test conditions potentially affecting biodegradation results. Based on Henry's law constant values, many of the category members are expected to be fairly volatile. It is not clear from the available information that precautions were taken in all studies to prevent loss of substrate through volatilization. Thus, volatile losses may have contributed to the observed variability.

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

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As far as structural features, carbon number would be expected to play a role in biodegradation from both solubility/bioavailability and steric effects. There is no clear correlation between carbon number and degree of biodegradation for alpha olefins. The internal olefins may exhibit increasing biodegradation with increasing carbon number, up to C<sub>24</sub> (compare the C<sub>20</sub>-C<sub>24</sub> with the C<sub>6</sub>-C<sub>12</sub> results in Table 6). Overall, the data suggest double bond location to be more important than carbon number. Theoretically, the branched olefins might be expected to be less biodegradable. However, the existing data do not support this supposition. Testing in an OECD 301B test with a C<sub>20</sub>-C<sub>24</sub> branched and linear material (>70% branched) resulted in 92% degradation in 28 days. Both substrate and benzoate showed unusually high percent biodegradation (92 and nearly 100 %, respectively), suggesting some bias in the test. However, since both substrate and benzoate were biased the same way, the test still supports ready biodegradability of the substrate.

Location of the double bond in the alpha versus an internal position appears to play a role in biodegradability. The C<sub>6</sub>-C<sub>12</sub> internal olefins have a lower percentage biodegradation while the higher carbon numbered internal olefins have, generally, a greater percent biodegradation (Table 6). Alpha olefin biodegradation appears to be insensitive to carbon number across the range tested. One literature source of general olefin biodegradability information makes a statement that the alpha olefins are favoured over internal olefins (Pitter and Chudoba, 1990). This publication tabulates BOD/ThOD (Theoretical Oxygen Demand) data for example olefins, but the data do not support the text's statement since all the ratios fall in the same range.

A variety of OECD and ISO methods were used in the testing. The lower C<sub>6</sub>-C<sub>14</sub> internal olefins were tested with 301F, while the C<sub>16</sub> and greater were tested by other methods. All are acceptable methods, but this variety could account for some of the variability in the results. However, review of the test conditions, as summarized in the robust summaries, does not highlight any systematic effects. The poor solubility of C<sub>8</sub> and higher olefins makes bioavailability a potential factor if the mass transfer effects impede biodegradation rates. However, most test conditions used either steady agitation or some form of dispersing medium to enhance solubilization during the test period. As far as test method effects are concerned, the source of inoculum is probably the greatest, and least controllable, source of variation.

Additional estimates of aerobic biodegradability of the members of the Higher Olefins Category were obtained using BIOWIN (versions 4.00 and 4.01), a subroutine of the computer program EPIWIN (EPIWIN, 2000a, b). With the exception of "C<sub>10,12</sub> olefin rich hydrocarbons" and "C<sub>12,14</sub> olefin rich hydrocarbons," the BIOWIN estimations are generally consistent across carbon numbers through C<sub>18</sub> and show "fast" biodegradation in all four models through C<sub>24</sub>, with primary degradation predicted to occur in days for C<sub>6</sub>-C<sub>18</sub> olefins, in "days to weeks" for C<sub>20</sub>-C<sub>30</sub> olefins, and in "weeks" for C<sub>54</sub> olefins. "Ultimate biodegradation" was predicted to occur in "days to weeks" or "weeks" for C<sub>6</sub> to C<sub>24</sub> olefins, in "weeks to months" for C<sub>26</sub>-C<sub>30</sub> olefins, and in "months" for C<sub>54</sub> olefins. The prediction for primary degradation ("days to weeks") for "C<sub>10,12</sub> olefin rich hydrocarbons," which was modelled using a structure with double bonds in five locations, was different from those for C<sub>10</sub> and C<sub>12</sub> alpha and internal olefins; and the MITI models predicted that the "C<sub>10,12</sub> olefin rich hydrocarbons" and "C<sub>12,14</sub> olefin rich hydrocarbons" would not biodegrade fast.

### Conclusions

- The weight of evidence shows that members of the Higher Olefins Category have the potential for degradation in the environment.
- Bond location appears to play a role in biodegradability, with alpha olefins showing higher degradability than internal olefins; however, available data are not clearly correlated with carbon number or any other identifiable parameter.

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

- Test protocols vary, but no systematic bias in results can be observed from the data presented. Inadequately controlled loss of substrate through volatilization may have contributed to the observed variability.
- Testing higher carbon numbers in the C<sub>24</sub>-C<sub>54</sub> range would encounter some mass transfer limitation effect due to solubility, which would in turn reduce biodegradability results.
- Sufficient data are available to assess the potential biodegradability of this category.

**Table 6** Summary of ready biodegradability tests for members of the Higher Olefins Category (shaded rows) and surrogate chemicals (C<sub>6</sub> – C<sub>30</sub> alkenes)<sup>a</sup>

Chemical Substance	Alpha/Internal (AO/IO)	Method	Biodegradation at 28 Days (%)	Pass (P)/Fail (F) for Ready Biodegradation
CAS No. 592-41-6, 1-Hexene	AO	301C O2	77	P <sup>d</sup>
CAS No. 592-41-6, 1-Hexene	AO	Closed Sturm CO2	22	F
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 602-57-1, 1-Heptene	IO	301C O2	72	P <sup>e</sup>
CAS No. 85535-87-1, Alkenes C10-13	IO	301D O2	65-70	F <sup>e</sup>
CAS No. 85535-87-1, Alkenes C10-13	IO	301D O2	60-67	F <sup>e</sup>
CAS No. 1120-36-1, 1-Tetradecene	AO	301D O2	62-65	F <sup>e</sup>
CAS No. 1120-36-1, 1-Tetradecene	AO	301B CO2	48-56	F
CAS No. 1120-36-1, 1-Tetradecene	AO	301C O2	52	P <sup>e</sup>
CAS No. 1120-36-1, 1-Tetradecene	AO	301B CO2	39-48	F
CAS No. 1120-36-1, 1-Tetradecene	AO	301B CO2	47-53	F
CAS No. 26952-14-7, Hexadecene; CAS No. 27070-58-2, Octadecene	IO	ISO Marine BODIS O2	48	F
CAS Nos. 182636-03-9, 182636-04-0, and 182636-05-1; C20-24 Alkenes, branched and linear	IO	301B CO2	92	P <sup>c</sup>
CAS Nos. 182636-05-1; 182636-06-2, 182636-08-4;	IO	301B CO2	51	F

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical Substance	Alpha/Internal (AO/IO)	Method	Biodegradation at 28 Days (%)	Pass (P)/Fail (F) for Ready Biodegradation
C24-30 Alkenes, branched and linear				

<sup>a</sup> Study details and references are found in the robust summaries in the dossiers.

<sup>b</sup> Member of Higher Olefins Category

<sup>c</sup> Passed: Met criteria for "ready biodegradability" by achieving 60% degradation within the 10-day window.

<sup>d</sup> Passed: This is a MITI Test and the 10-day window criterion does not apply.

<sup>e</sup> Failed because it is not known whether 60% biodegradation was achieved within the 10-day window.

<sup>f</sup> Failed because 60% biodegradation was not achieved within the 10-day window.

### 2.2.6 Bioaccumulation

Based on the model predictions of the BCF (bioconcentration factor) subroutine (version 2.14 or 2.15) of the computer program EPIWIN (version 3.10 or 3.11; EPIWIN, 2000a, b), the C<sub>6</sub>-C<sub>7</sub> and C<sub>16</sub>-C<sub>54</sub> Higher Olefins Category members are not expected to bioaccumulate. Although the C<sub>8</sub>-C<sub>15</sub> olefins have BCFs >250 and K<sub>ow</sub> values ranging from 4.13 to 7.49, and thus are considered to have the potential for bioaccumulation, their physico-chemical properties and fate indicate that there would be limited environmental exposure because of volatility, biodegradability and limited solubility. The estimated BCFs are shown in Table 7.

**Table 7** Calculated bioconcentration factors (BCF) for C<sub>6</sub>-C<sub>54</sub> alpha (A) and/or internal (I) olefins<sup>a</sup>

	C6 (I/ neohexene)	C7 (I)	C8 (I)	C9 (I)	C10 (A/I)	C11 (I)	C12 (A/I)	C13(A/I)	C14 (A/I)	C15 (I)	C16 (A/I)	C18 (A and I) and C20- C54 (A)
<b>BCF</b>	46/44	236	659	632	489/489	361	313/314	748/748	1584/2030	431	71/92	3.2 - 4.6

<sup>a</sup> Calculation details and references are found in the robust summaries in the dossiers.

### 2.2.7 Other Information on Environmental Fate

No data available

## 2.3 Human Exposure

### 2.3.1 Occupational Exposure

No governmental occupational exposure standards are available for any of the substances within the category (ACGIH, 2003). However, one company reported an internal standard of 100 ppm for hexene and octene (343 and 458 mg/m<sup>3</sup> respectively). Members of the Higher Olefins Category are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals (to include polymers). C<sub>12</sub>-C<sub>20</sub> olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. C<sub>20</sub>-C<sub>54</sub> alpha olefins are used in wax applications. No other non-intermediate applications have been identified. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. Should these exposures occur, then the potential for exposure via the inhalation route would decrease as the carbon number increases due to the subsequent increase in boiling point and decrease in vapor pressure. Furthermore, it is a common practice to use personal protective equipment. In the case of dermal exposures, protective gloves

would be worn with C<sub>18</sub> and lower molecular weight substances due to the mildly irritating properties of these chemicals (ACC Higher Olefins Panel, 2002).

### 2.3.2 Consumer Exposure

None of the compounds within the category were identified on the National Library of Medicine Household Products Database (NLM, 2003b). The primary intended use of the chemicals in this category is in the synthesis of other industrial chemicals. Therefore, consumer exposure is limited to waxes containing C<sub>20</sub>-C<sub>54</sub> alpha olefins.

## 3 HUMAN HEALTH HAZARDS

### 3.1 Effects on Human Health

The exposure routes of concern for human health are considered to be dermal and inhalation. Data presented in the Category Summary are considered the key studies to describe the hazards of these compounds. All other data may be found in each individual chemical's respective dossier.

#### 3.1.1 Toxicokinetics, Metabolism and Distribution

Studies with several alpha or internal olefins spanning the range from C<sub>6</sub> to C<sub>16</sub> indicate 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 (Watabe and Yamada, 1975; Maynert et al., 1970; Oesch, 1973; Watabe and Maynert, 1968). The latter two metabolites are likely to be excreted in urine as mercapturic acids (Sipes and Gandolfi, 1991).

Effects seen in repeated-dose studies with C<sub>6</sub>, C<sub>8</sub>, and C<sub>14</sub> alpha olefins and C<sub>6</sub>, C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> internal olefins (see Section 3.1.5) indicate that these olefins are absorbed by the blood and reach the liver and kidneys following oral or inhalation exposure. Studies of the toxicokinetic properties of inhaled C<sub>2</sub>-C<sub>10</sub> alpha olefins confirm that, within the carbon number range tested, absorption of these alkenes occurs and that the alkenes accumulate in the brain, liver, kidneys and perirenal fat, with the concentrations increasing with the number of carbon atoms (Eide et al., 1995; Zahlisen et al., 1993). In contrast, studies in rats with structurally similar C<sub>14</sub>-C<sub>30</sub> alkanes run concurrently with a C<sub>18</sub> alpha olefin and a C<sub>19</sub> internal olefin indicate that alkenes having more than 29 carbon atoms would not be absorbed to a significant extent (Albro and Fishbein, 1970).

#### Studies in Animals

##### *In vivo Studies*

Absorption, distribution and elimination were studied in the rat after inhalation of individual C<sub>2</sub>-C<sub>8</sub> 1-alkenes at 300 ppm, 12 hr/day for 3 consecutive days (Eide et al., 1995). Concentrations of olefins measured in blood, lung, brain, liver, kidney and perirenal fat reached steady state levels after the first 12 hr of exposure, and concentrations 12 hr after the last exposure were generally low (<3% of the concentrations immediately after exposure), except in the fat. Concentrations of 1-alkenes in blood and tissues increased with increasing number of carbon atoms (see Table 8).

The toxicokinetic properties of C<sub>8</sub>-C<sub>10</sub> 1-alkenes were studied in the rat after inhalation of individual alkenes at 100 ppm, 12 hr/day for 3 consecutive days (Zahlisen et al., 1993). Concentrations of olefins were measured in blood, brain, liver, kidney and perirenal fat immediately after each exposure and 12 hr after the third exposure. The 1-alkenes showed an efficient absorption to blood combined with accumulation in organs, with the concentration increasing with number of

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

carbon atoms. After the 12-hour recovery period, very little 1-alkene was found in blood, brain, liver or kidney; but the concentrations of C<sub>8</sub>, C<sub>9</sub> and C<sub>10</sub> 1-alkenes in fat were 31, 46 and 66%, respectively, of the concentrations on Day 3 (see Table 9).

**Table 8** Concentrations of individual 1-alkenes after the third daily 12 hr inhalation exposure of rats to 300 ppm and concentrations in fat 12 hr after the third exposure (n=4) (Eide et al., 1995)<sup>a</sup>

Chemical	Blood	Liver	Lung	Brain	Kidneys	Fat	Fat 12 hr after 3 <sup>rd</sup> exposure
Ethene	0.3	0.4	2.3	0.7	0.7	7	nd
Propene	1.1	0.3	2.9	1.7	1.8	36	nd
1-Butene	1.9	0.8	4.9	3.0	5.7	70	0.3
1-Pentene	8.6	51.6	31.4	41.0	105.7	368	19
1-Hexene	18.2	66.8	59.7	59.7	188.0	1031	77
1-Heptene	37.0	138.3	85.6	109.3	269.3	2598	293
1-Octene	60.1	443.7	202.4	270.0	385.1	4621	943

<sup>a</sup> All concentrations are in μmol/kg; nd = not detectable (detection limits not provided)

**Table 9** Concentrations of individual 1-alkenes after the third daily 12 hr inhalation exposure of rats to 100 ppm and after 12 hr recovery (n=4) (Zahlsen et al., 1993)<sup>a</sup>

	1-Octene		1-Nonene		1-Decene	
	After third exposure	After 12 hr recovery	After third exposure	After 12 hr recovery	After third exposure	After 12 hr recovery
Blood	12.4	0.1	15.9	0.4	16.4	0.7
Brain	69.7	0.5	116.3	2.7	138.1	6.3
Liver	78.9	nd	130.4	1.1	192.8	4.0
Kidney	139.3	0.9	146.7	4.6	162.0	9.3
Fat	720	226	2068	953	2986	1971

<sup>a</sup> All concentrations are in μmol/kg; nd = not detectable (limit of detection varied between substances and organs: in blood and organs generally within range from 0.1 – 1 μmol/kg; in fat from 5 – 10 μmol/kg)

Another *in vivo* experiment was conducted to determine whether the olefinic double bond is implicated as a participant in the NADPH-dependent destructive interaction of olefins with the P-450 enzyme (Ortiz de Montellano and Mico, 1980). Phenobarbital-treated rats were injected with 1-heptene, *cis* and *trans* 2-nonene, 4-ethyl-1-hexene, and 3-methyl-1-octene. Four hours after treatment, the livers were analyzed for the presence of abnormal hepatic pigments. These pigments have been shown to be porphyrins derived from the prosthetic heme moiety of inactivated P-450 enzymes. Hepatic green pigments were formed after administration of 4-ethyl-1-hexene, 3-methyl-1-octene and 1-heptene. The *cis*- and *trans*-2-nonenes produced no abnormal pigments.

Albro and Fishbein (1970) studied the influence of carbon number on the absorption of orally administered C<sub>14</sub>-C<sub>30</sub> alkanes by male rats. Individual hydrocarbons were administered intragastrically, and the percentage retained was calculated as the material not excreted in feces within 4 days. An inverse relationship between carbon number and absorption following oral administration of C<sub>14</sub>-C<sub>30</sub> alkanes was reported, and the authors concluded that alkanes having more than 29 carbon atoms would not be absorbed to a significant extent. In additional experiments in which, among other hydrocarbons, 1-octadecene, and cis- and trans-nonadecene were tested, Albro and Fishbein (1970) demonstrated that the relationship also applied to branched, cyclic and unsaturated hydrocarbons; i.e., carbon number appeared to be the determining factor in retention under the conditions tested. de Rooij et al. (1993) reported that analysis of hydrocarbon residues in livers of rats fed a range of mineral oils or waxes in 90-day studies showed no absorption of hydrocarbons of chain length >C<sub>35</sub>. The higher carbon number reported in this study compared to that reported by Albro and Fishbein (1970) may reflect the long term exposure which enabled the detection of accumulated material from low level absorption.

#### *In vitro Studies*

1-Hexene was tested in an *in vitro* system and was demonstrated to cause the autocatalytic destruction of cytochrome P-450 and heme in hepatic microsomes from phenobarbital pretreated rats (Shell Development Company, 1984).

In the presence of rat liver microsomes and NADPH, n-1-octene, n-4-octene and 3-ethyl-2-pentene were converted to the glycols with no trace of epoxide (Maynert et al., 1970). The relative yields of the glycols (11.3%, 4.0%, 0.12%) indicate that increasing substitution of the ethylenic moiety by alkyl groups decreases the rate of the reaction. In the presence of the epoxide hydrolase inhibitor, 4,5-epoxy-n-octane, the product from 10 μmoles n-1-octene contained 1,2-epoxy-n-octane (0.40 μmoles) and n-octane-1, 2-diol (0.23 μmoles), whereas in the absence of the inhibitor, only the glycol (0.64 μmoles) could be detected. In the presence of 1,2-epoxy-n-octane, the substrate n-4-octene produced the epoxide but not the glycol. The authors concluded that it is likely that the biological conversion of the alkenes proceeds through epoxides.

1-Heptene, 2-nonene, 3-hexene, 4-ethyl-1-hexene, 3,3-dimethyl-1-hexene, 3-methyl-1-octene and 2-methyl-1-heptene were tested in an *in vitro* experiment in which hepatic microsomes from phenobarbital-pretreated rats were incubated with NADPH and analyzed for the presence of cytochrome P-450 (Ortiz de Montellano and Mico, 1980). Hepatic microsomal cytochrome P-450 was destroyed *in vitro*, in the presence of NADPH, by 4-ethyl-1-hexene, 3-methyl-1-octene, 2-nonene and 1-heptene. The cis- and trans-2-nonenes exhibited marginal destructive activity (10% loss after 30 minutes). No significant cytochrome P-450 loss was observed after incubation with 2-methyl-1-heptene, 3,3-dimethyl-1-hexene or 3-hexene, suggesting that steric and electronic factors can suppress the destructive interaction. The epoxides of 3 of the terminal olefin substrates were synthesized and shown not to intervene in destruction of the enzyme by the parent olefins.

1-Hexadecene and an epoxide hydrolase inhibitor, 1,2-epoxydecane, were incubated with rabbit liver microsomes and an extract was analyzed (Watabe and Yamada, 1975). The formation of the epoxide (1,2-epoxyhexadecane) was observed only when the olefin was incubated in the presence of the epoxide hydrolase inhibitor. In the absence of inhibitor, 1,2-dihydroxyhexadecane was formed. The authors concluded these results indicate that 1-hexadecene is metabolized to 1,2-dihydroxyhexadecane via 1,2-epoxyhexadecane.

#### Conclusion

Metabolism of Higher Olefins Category members occurs in hepatic endoplasmic reticulum via initial formation of a transient epoxide, which is further metabolized to the corresponding glycol or

conjugated with glutathione. The latter two metabolites are expected to be excreted in urine as mercapturic acids.

Following oral or inhalation exposure, category members up to about C<sub>30</sub> are expected to be absorbed by the blood and to accumulate in the brain, liver, kidneys and perirenal fat, with the concentration increasing with the number of carbon atoms through C<sub>10</sub>, and then decreasing with carbon number after C<sub>14</sub>. The increased retention in fat of alkenes with higher carbon numbers is presumably a function of their increased lipophilicity, and decreased likelihood to be exhaled unchanged, compared to the lower volatile alkenes. Since unchanged alkenes are not considered to be toxic, and because tissue levels rapidly clear after exposure ceases, absorption of members of the Higher Olefins Category is unlikely to have any biologically significant effect.

### 3.1.2 Acute Toxicity

Results of the acute studies, summarized in the Annex, Table 2, indicate that alkenes ranging in carbon number from C<sub>6</sub> to C<sub>54</sub>, alpha and internal, linear and branched, demonstrate low acute toxicity by the oral, inhalation and dermal routes of exposure: Rat oral LD<sub>50</sub> >5 g/kg; rat 4-hr inhalation LC<sub>50</sub> range = 110 mg/L (32,000 ppm) to 6.4 mg/L (693 ppm) for C<sub>6</sub> to C<sub>16</sub>; and rat/rabbit dermal LD<sub>50</sub> > highest doses tested (1.43-10 g/kg).

#### Studies in Animals

##### *Inhalation*

By the inhalation route in rats, mice and guinea pigs, results of many studies with C<sub>6</sub>-C<sub>16</sub> alpha and internal olefins show that median lethal concentration values (LC<sub>50</sub>) are greater than the saturated mist concentration or a vapour concentration limited by the Lower Explosive Limit (LEL). The rat 4-hr inhalation LC<sub>50</sub> range is 110 mg/L (32,000 ppm) to 6.4 mg/L (693 ppm) for C<sub>6</sub> to C<sub>16</sub> alpha or internal olefins.

##### *Dermal*

Many studies with alpha and internal olefins ranging from C<sub>6</sub>-C<sub>26</sub> show that the median lethal dose values (LD<sub>50</sub>) for the dermal route of exposure in rabbits are greater than the highest doses tested, which ranged from 1.43 g/kg to 10 g/kg. Similarly, the dermal LD<sub>50</sub> values for rats exposed to a C<sub>12</sub>, C<sub>13</sub>, C<sub>20</sub>-C<sub>24</sub> or C<sub>24</sub>-C<sub>54</sub> alpha olefin, a C<sub>10</sub>-C<sub>13</sub> internal olefin, or a C<sub>20</sub>-C<sub>24</sub> internal (branched and linear) olefin, are greater than the highest doses tested (2-10 g/kg).

##### *Oral*

Many studies with C<sub>6</sub>-C<sub>54</sub> alpha and internal olefins show that the median lethal dose values (LD<sub>50</sub>) for the oral route of exposure in rats are greater than 5 g/kg; and, in those studies in which the highest dose tested was 10 g/kg, the LD<sub>50</sub> was found to be greater than 10 g/kg.

#### Studies in Humans

##### *Inhalation*

In a review, Cavender (1998) noted that 1-hexene, when inhaled at a concentration of 0.1 percent (1000 ppm), causes central nervous system (CNS) depression with mucous membrane irritation, vertigo, vomiting and cyanosis.

## Conclusion

By the oral, dermal, and inhalation routes of exposure, the Higher Olefins Category members appear to have a low order of acute toxicity.

### 3.1.3 Irritation

The data for irritation are summarized in the Annex, Table 2a.

#### Skin Irritation

##### *Studies in Animals*

Skin irritation studies are available for C<sub>6</sub>-C<sub>24</sub> alpha and internal olefins. Most available data show that, under 4-hr semi-occluded conditions, C<sub>6</sub>-C<sub>18</sub> alpha and internal olefins and C<sub>20</sub>-C<sub>24</sub> alpha olefins are only mildly irritating to rabbit skin (see the Annex, Table 2a). When current testing guideline recommendations were used, only two of the products tested (C<sub>10</sub> and C<sub>12</sub> alpha olefins) produced 24-72 hr scores for erythema or edema  $\geq 2$ . When tested under more extreme conditions (24-hr exposure, abraded skin, occluded dressing), several alpha and internal olefins caused irritation. In a 4-hr semi-occluded study in rabbits with a C<sub>20</sub>-C<sub>24</sub> internal olefin, all scores were zero.

In a repeated dose study, 1-hexadecene was administered to skin of guinea pigs on 4 alternate days during 7 days at 0.5-0.6 ml/day and skin evaluations were made every other day for 20 days following the first treatment (Hoekstra and Phillips, 1963). The report does not indicate that the treated site was covered or cleaned between or after applications. Skin irritancy was graded on a 0-8 scale. 1-Hexadecene was severely irritating with a maximum score of 8.

##### *Studies in Humans*

A human patch test was performed with 1-octadecene (Shell Oil Company, 1992a). Each volunteer received a single 24-hour semi-occluded patch exposure to undiluted material and to dilutions in mineral oil (25%, 10% and 1%). No evidence of irritation was noted with dilute applications, but strong clinical reactions were produced by the undiluted 1-octadecene.

#### Eye Irritation

##### *Studies in Animals*

Eye irritation studies with C<sub>6</sub>-C<sub>24</sub> alpha and/or internal olefins indicate that these chemicals are only slightly irritating to rabbit eyes (see the Annex, Table 2a).

#### Respiratory Tract Irritation

##### *Studies in Animals*

No animal studies have been identified for this endpoint.

##### *Studies in Humans*

In a review, Cavender (1998) noted that 1-hexene, when inhaled at a concentration of 0.1 percent (1000 ppm), causes mucous membrane irritation; however, there is no evidence that 1-hexene or any C<sub>6</sub>-C<sub>54</sub> alpha or internal olefin causes serious respiratory irritation.

## Conclusion

Based on available data, exposure to category members may cause mild skin and eye irritation and inhalation of the lower chain length members may cause mild respiratory tract irritation. Prolonged exposure of the skin for many hours may cause skin irritation.

### 3.1.4 Sensitization

The available data for sensitization are summarized in the Annex, Table 2a.

#### Studies in Animals

##### *Skin*

Available data for C<sub>6</sub>-C<sub>24</sub> alpha and internal olefins indicate that these materials do not cause skin sensitization in guinea pigs.

##### *Respiratory Tract*

No data were identified for this endpoint.

#### Studies in Humans

##### *Skin*

Thirty-six human volunteers received nine induction exposures (24-hr, semi-occluded patch on upper arm) to a 25% dilution of 1-octadecene in mineral oil (Shell Oil Company, 1992b). Challenge applications failed to elicit sensitization reactions.

##### *Respiratory Tract*

No data were identified for this endpoint.

## Conclusion

Based on data provided, members of the Higher Olefins Category are not likely to be skin sensitizers.

### 3.1.5 Repeated Dose Toxicity

Similar low levels of toxicity were demonstrated in several rat oral repeated dose studies with structural analogues of members of the Higher Olefins Category. The substances tested were: C<sub>6</sub>, C<sub>8</sub> and C<sub>14</sub> linear alpha olefins, C<sub>6</sub> internal olefin (58% branched), C<sub>16</sub>/C<sub>18</sub> internal olefins (26% branched), C<sub>18</sub> internal olefin (32.5% branched) and C<sub>20</sub>-C<sub>24</sub> internal olefins (>70% branched). When tested in rats by the inhalation route, 1-hexene, a structural analogue of hexene (the category member with the highest vapour pressure), produced only reduced bodyweight in females and questionable organ weight changes. Data also exist for a short-term (14 days) dermal study in rats (C<sub>12</sub>-C<sub>16</sub> alpha olefin blend). The data for repeated dose toxicity are summarized in the Annex, Table 2.

#### Studies in Animals

##### *Inhalation*

1-hexene: A subchronic study of 1-hexene was conducted by inhalation, considered to be the most relevant route for human repeated exposure (Gingell et al., 1999). Rats were exposed to 0, 300,

1000, and 3000 ppm (0, 1.03, 3.44, and 10.33 mg/L) 1-hexene for 90 days (6 hrs/day, 5 days/week) and evaluated for systemic toxicity. No mortalities and no clinical signs of toxicity attributable to 1-hexene exposures were observed. Female rats exposed to 3000 ppm had significantly lower body weights. Several statistically significant effects in hematology, clinical chemistry, and urinalysis evaluations were observed: elevated serum phosphorus in males at 300, 1000 and 3000 ppm and in females at 1000 and 3000 ppm; lower serum lactate dehydrogenase in female rats exposed to 1000 ppm, and in both male and female rats exposed to 3000 ppm; lower serum albumin in female rats exposed to 3000 ppm; elevated hematocrit and RBC count in 3000 ppm males and in 1000 and 3000 ppm females; lower mean corpuscular hemoglobin and hemoglobin concentration in 1000 and 3000 ppm females. These findings were either of small magnitude or did not correlate with histopathological findings, and thus did not appear to be of biological significance. At 3000 ppm, male rats exhibited slightly increased absolute and relative testicular weights; however, when the left testicle was detunicated prior to weighing, there was no statistically significant increase in testis weight compared with the controls. Female rats had slightly decreased absolute (but not relative) liver and kidney weights, at 3000 ppm. No treatment-related gross or histological lesions were noted in these or other tissues. Sperm counts were observed and were not considered to show statistical significance. Exposure to 1-hexene did not affect neuromuscular coordination in females as determined using the Rotorod. The NOEL appeared to be 3.44 mg/L (1000 ppm), based on changes in body weight and questionable organ weight changes at 10.33 mg/L (3000 ppm). The LOEL was 10.33 mg/L (3000 ppm).

#### *Dermal*

C<sub>12</sub>-C<sub>16</sub> alpha olefins: A blend of C<sub>12</sub>-C<sub>16</sub> alpha olefins was administered to skin of rats once daily for nine applications in a two-week period at 2.0 g/kg (undiluted) and 1.0 g/kg (diluted 1:1 with corn oil) (Gulf Life Science Center, 1983a). All animals survived to the end of the study and no moribund animals were observed during the study. The high dose produced severe skin reactions in all animals. Dermal reactions increased in severity with the number of applications. When the test material was administered at a 1.0 g/kg level, slight skin reactions were seen. Depressed body weight gains were observed in the 2.0 g/kg group but not in the 1.0 g/kg group. The decreases in bodyweight were associated with decreases in the absolute weights of most organ systems and small but statistically significant differences in the relative weight ratios for several organs. No treatment-related effects were noted for food consumption, clinical signs (other than dermal reactions), hematology, or clinical chemistry. Treatment was associated with histological changes in the skin at the point of application in all animals, but there were no other microscopic changes seen that could be associated with the test substance. Study authors concluded that, under conditions of the study, repeated dermal applications of the blend of C<sub>12</sub>-C<sub>16</sub> alpha olefins at 2.0 g/kg, but not at 1.0 g/kg, caused severe skin reactions and depressed body weight gains. The reviewer assessed NOAEL for systemic effects was 1.0 g/kg/day and the LOAEL was 2.0 g/kg/day, based on decreased body and organ weights.

#### *Oral*

alkenes, C<sub>6</sub> (internal, 58% branched): Rats were orally dosed with alkenes, C<sub>6</sub> (OECD 422 combined repeated dose toxicity and reproduction/developmental toxicity screening test) at concentrations of 0, 100, 500 or 1000 mg/kg/day (Thorsrud, 2003a). The reproduction/developmental toxicity results from this study are discussed in Section 3.1.8; and the neurotoxicity results are discussed in Section 3.1.9. There were no toxicologically meaningful differences noted in mean body weights, body weight gain, food consumption, hematology, coagulation or the clinical chemistry parameters evaluated. In males, statistically significant differences in organ weight data included higher absolute adrenal weight in the 100 mg/kg/day group; higher absolute kidney weights in the 100, 500 and 1000 mg/kg/day groups; higher kidney weight relative to final

body weight in the 500 and 1000 mg/kg/day groups; and higher liver weight relative to final body weight in the 1000 mg/kg/day group. In females, statistically significant differences in organ weight data included higher kidney weight relative to final body weight in the 500 and 1000 mg/kg/day groups, and higher liver weight relative to final body weight in the 1000 mg/kg/day group. None of the differences was considered toxicologically meaningful since they did not correlate with any toxicologically significant histopathological changes. Minimal to mild hyaline droplet nephropathy within the proximal convoluted tubules were observed in males in the 1000 mg/kg/day group; however, the author concluded that these findings are not considered toxicologically significant to humans. The NOAEL was determined to be 1000 mg/kg/day. The NOEL for systemic toxicity was 100 mg/kg/day for females (kidney effects). No NOEL was determined for males due to kidney and adrenal effects. The LOEL was 500 mg/kg/day for females and 100 mg/kg/day for males.

1-hexene: Groups of 5 male and 5 female rats were exposed to 1-hexene via gavage for 28 days at 0, 10, 101, 1010 and 3365 mg/kg/day (OECD Test Method 407) (Dotti et al., 1994). The main effect exhibited was irritation of the gastric mucosa at the two top dose levels ( $\geq 1010$  mg/kg/day) along with reduced body weights. Spleen weights were reduced at the top dose of 3365 mg/kg/day, but there were no associated histological findings. Pathological changes were restricted to gastric effects. The NOEL for the study was determined to be 101 mg/kg/day for males (male-rat specific kidney effect) and 1010 mg/kg/day for females. The LOEL was 3365 mg/kg/day for females and 1010 mg/kg/day for males.

1-hexene: Gingell et al. (2000) conducted a reproduction/developmental toxicity screening study (OECD 421) in rats with 1-hexene (gavage at doses of 0, 100, 500 and 1000 mg/kg/day). The reproductive and developmental toxicity results are discussed in Section 3.1.8. Male rats were dosed for 44 consecutive days and females were dosed for 41-55 consecutive days. No effects were observed in females. The following kidney effects were observed in males: pitted kidneys (2/12 in 500 mg/kg/day group and 3/12 in the 1000 mg/kg/day group); and the accumulation of eosinophilic hyaline droplets in the proximal convoluted tubules in all treated rats (incidence of 0/12, 7/12, 8/12 and 9/12 for the 0, 100, 500 and 1000 mg/kg/day groups). The extent of hyaline droplet formation also increased with dose. Although there was no immunohistochemical verification, the authors concluded that the formed droplets were  $\alpha_2\mu$ -globulin, specific to male rats. The NOEL for males was  $<100$  mg/kg/day and the LOEL was 100 mg/kg/day. The NOEL for females was 1000 mg/kg/day.

1-octene: Four groups of 20 male and 20 female rats were dosed via gavage with 1-octene for 90 days at 0, 5, 50, and 500 mg/kg/day (Til et al., 1986). Changes that were considered treatment-related occurred only in the high-dose group. They consisted of increased kidney weights (in both sexes), histopathological renal changes (males only), decreased plasma chloride (in both sexes), and increased plasma creatinine concentration (females only). These findings indicate a nephrotoxic effect at 500 mg/kg/day. The authors of the study concluded the NOEL to be between 50 and 500 mg/kg/day and probably only slightly less than 500 mg/kg/day. The authors' rationale was based on only slight changes being observed at 500 mg/kg/day and no-treatment related effects being observed at the next lower dose of 50 mg/kg/day. When compared to the control group there were no significant differences in body weight, food intake, signs of toxicity or behavioral abnormalities, which could be related to the test substance. Upon review of the study, it appears that the only NOEL demonstrated from the data is 50 mg/kg/day. This conclusion is based on the limitations of the doses utilized in the study design and treatment-related effects that were observed at 500 mg/kg/day. The LOEL was 500 mg/kg/day.

1-tetradecene: Rats were orally dosed with 1-tetradecene (OECD modified 422, combined repeated dose toxicity and reproduction/developmental toxicity screening test) at concentrations of 0, 100, 500, and 1000 mg/kg/day (Daniel, 1995). (The reproductive/developmental toxicity results from

this study are discussed in Section 3.1.8; and the neurotoxicity results are discussed in Section 3.1.9.). An increased incidence of minimal-to-mild hepatocyte cytoplasmic vacuolation, associated with increased liver weights, was observed in both sexes at  $\geq 500$  mg/kg/day, with the distribution being inconsistent (multifocal, centrilobular, periportal, generalized). Pitted kidneys and an accumulation of hyaline droplets in the proximal convoluted tubules of the kidneys occurred in males at all dose levels. The kidney effects were interpreted to be a result of hydrocarbon nephropathy, which is specific to male rats. The NOEL for females was 100 mg/kg/day (liver effects). A NOEL for systemic toxicity to the males was not determined due to the hydrocarbon nephropathy. The LOEL was 500 mg/kg/day for females and 100 mg/kg/day for males.

C<sub>16</sub>/C<sub>18</sub> internal linear and branched olefin (26% branched): Rats were orally dosed with a C<sub>16</sub>/C<sub>18</sub> internal linear and branched olefin (OECD 407) at concentrations of 0, 25, 150 or 1000 mg/kg/day for 4 weeks (Clubb, 2000). Functional observations were performed for neurotoxicity evaluation (see Section 3.1.9). There was little evidence of toxicity noted in animals treated at levels up to 1000 mg/kg/day. A slight increase in male body weight was noted at 1000 mg/kg but the increase did not achieve statistical significance. Statistically significant, but equivocal, changes in urinary volume (higher than controls) and kidney weight (lower than controls) were considered unlikely to be treatment-related in the absence of any macro- or microscopic changes. There were no treatment-related findings associated with treatment at 25 or 150 mg/kg/day. The NOAEL was 1000 mg/kg/day.

C<sub>18</sub> internal linear and branched olefin (32.5% branched): In a combined reproduction/developmental toxicity screening test (OECD 421), a C<sub>18</sub> internal linear and branched olefin was administered by gavage to rats at doses of 0, 100, 500 and 1000 mg/kg/day (Thorsrud, 2003b). The reproductive and developmental toxicity results are discussed in Section 3.1.8. General toxicity endpoints were limited to mortality, clinical observations, bodyweight, food consumption, gross necropsy examination, and reproductive organ weights and histopathology. The NOAEL was 1000 mg/kg/day.

C<sub>20</sub>-C<sub>24</sub> internal branched and linear olefins (>70% branched): The test material was administered by gavage to rats at 0, 100, 500 and 1000 mg/kg/day for a period of 13 weeks (OECD 408) (Brooker, 1999). At the end of the 13-week treatment period, 10 male and 10 female animals from the control and high dose groups were maintained, undosed for a 4-week period to assess recovery. There were no deaths during the study. No clinical signs or effects on bodyweight or food intake were seen. No ophthalmological or neurobehavioral effects were noted (see Section 3.1.9 for a discussion of the neurobehavioral screen). Slight yet reversible changes in hematological parameters were noted amongst animals receiving 1000 mg/kg/day. Group mean glucose levels were significantly higher amongst male rats receiving 500 and 1000 mg/kg/day. Minimal, adaptive hepatic changes (centrilobular hepatocyte hypertrophy), associated with higher group mean liver weight, were detected in a small number of females of all treated groups, but was statistically significant only at 1000 mg/kg/day. An increased incidence of minimal or slight adrenal cortical hypertrophy was noted amongst females receiving 1000 mg/kg/day associated with increased adrenal weight. An increased incidence of minimal or slight epithelial hyperplasia in the stomach was noted amongst males receiving 1000 mg/kg/day. These findings were not present following a 4-week recovery period and were considered to be of no toxicological importance. The author assessed NOAEL was 1000 mg/kg/day. The NOEL was 100 mg/kg/day for males (glucose). The NOEL for females was 500 mg/kg/day (adrenal and liver effects). The LOEL was 500 mg/kg/day for males and 1000 mg/kg/day for females.

### Studies in Humans

No data were identified.

## Conclusion

Repeated dose studies in which rats were exposed by the inhalation route (C<sub>6</sub> alpha), dermal route (C<sub>12</sub>-C<sub>16</sub> alpha), or oral route (C<sub>6</sub> alpha and internal linear/branched; C<sub>8</sub> and C<sub>14</sub> alpha; and C<sub>16</sub>/C<sub>18</sub>, C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> internal linear/branched), have shown comparable levels of low toxicity. In females, alterations in body and organ weights, changes in certain clinical chemistry/hematology values, and liver effects were noted (NOELs of  $\geq 100$  mg/kg oral or  $\geq 3.44$  mg/L [1000 ppm] inhalation). In males, alterations in organ weights, changes in certain clinical chemistry/hematology values, liver effects, and kidney damage were noted (LOELs  $\geq 100$  mg/kg oral only). Male rat nephropathy was reported on oral administration of C<sub>6</sub>, C<sub>8</sub> and C<sub>14</sub> linear alpha olefins and C<sub>6</sub> internal olefins (58% branched), but was not seen in a study with C<sub>16</sub>/C<sub>18</sub> internal (26% branched) olefins or C<sub>20</sub>-C<sub>24</sub> branched and linear internal olefins (>70% branched). While no specific immunohistochemical staining was conducted to identify the hyaline droplets associated with the observed kidney effects, their morphology and occurrence only in male rats suggests that they are probably related to alpha<sub>2</sub> $\mu$ -globulin nephropathy, a male rat specific effect that is not considered relevant to human health (Hard et al., 1993; Baetcke et al., 1990). Slight increases in liver effects were seen in rat repeated dose oral studies with the C<sub>14</sub> and C<sub>20</sub>-C<sub>24</sub> alkenes (hepatocytic cytoplasmic vacuolation and associated increases in liver weights in males and females at high doses of 1-tetradecene, and centrilobular hepatocyte hypertrophy and associated increases in liver weights in females at high doses of C<sub>20</sub>-C<sub>24</sub> branched and linear internal olefins). Neither these findings nor other effects were present in the study with C<sub>20</sub>-C<sub>24</sub> branched and linear internal olefins following a 4-week recovery period, indicating reversibility of the observed effects; and no liver effects were noted in a study with C<sub>16</sub>/C<sub>18</sub> branched and linear internal olefins. Cytoplasmic vacuolation of hepatocytes is a common hepatic lesion in rodents, and may in part be an adaptive hypertrophic response to an intensified metabolic liver burden (Schulte-Hermann, 1974). It is generally considered to be caused by accumulation of glycogen and/or triglycerides; and it is possible that the effects are an indirect effect related to consumption of food, or to glycogen metabolism, rather than a direct toxic effect of the olefin.

### 3.1.6 Mutagenicity

Tests for gene mutation and chromosome aberrations exist for C<sub>6</sub> and C<sub>18</sub> linear alpha olefins (Huntingdon Research Center, 1990a, 1990b, 1990c; Dean, 1980; Shell Development Company, 1983a, 1983b, 1983c; Hazleton, 1982a; Gulf Life Sciences Center, 1983b, 1983c, 1983d), for C<sub>6</sub> (60-74% branched) (Exxon Biomedical Sciences, 1991a, 1991b, 1991c), C<sub>20</sub>-C<sub>24</sub> internal olefins (>70% branched) (Thompson, 1998a; Wright, 1998; Durward, 1998) and C<sub>24</sub>-C<sub>30</sub> internal olefins (>70% branched) (Thompson, 1998b), and for several of the homologues within those ranges. Based on the weight of evidence, these substances are not genotoxic. The available data for mutagenicity are summarized in the Annex, Table 2.

### *In vivo* Studies

Negative results were seen in bone marrow micronucleus tests in which mice were exposed via inhalation to 1000 - 25,000 ppm (3.44 - 86.05 mg/L) 1-hexene for 2 hrs/day for 2 days (Gulf Life Sciences, 1983b). Dermal application of a C<sub>12</sub>-C<sub>16</sub> blend of alpha olefins to mice also failed to induce an increase in micronucleated bone marrow erythrocytes (Gulf Life Sciences, 1983d). Via the oral route of exposure, weakly positive results were seen in a study with a C<sub>6</sub> branched internal olefin at 5 g/kg (Exxon Biomedical Sciences, 1991b), but this compound was negative when repeated via the inhalation route at 1057 ppm (3.64 mg/L, saturated vapours) for 6 hrs/day for 2 days (Exxon Biomedical Sciences, 1991c). Oral exposure studies with C<sub>6</sub>-C<sub>8</sub> (Exxon Chemical Company, 1993) and C<sub>8</sub>-C<sub>10</sub> branched internal olefins (Exxon Biomedical Sciences, 1991e) at 5

g/kg, and with a C<sub>16</sub> alpha olefin at 7.85 g/kg (Research Institute of Organic Synthesis, 1990), were negative. A micronucleus study with C<sub>20</sub>-C<sub>24</sub> linear and branched internal olefins at 2 g/kg via the intraperitoneal route of exposure was also negative (Durward, 1998). Evidence of bone marrow toxicity was observed only in the oral exposure studies with a C<sub>8</sub>-C<sub>10</sub> branched internal olefins and with a C<sub>16</sub> alpha olefin.

### *In vitro* Studies

The C<sub>6</sub>-C<sub>24</sub> alpha and internal olefins are not considered to be genotoxic as a result of a broad range of negative *in vitro* studies: bacterial reverse mutation (Exxon Biomedical Sciences, 1991a, 1991d; Huntingdon, 1990a; Hazleton, 1982a; Shell Development Company, 1983b; Brooks et al., 1983; Burghardtova et al., 1984; Dean, 1980; Research Institute of Organic Synthesis, 1990; and Thompson 1998a, 1998b); mitotic gene conversion in yeast (Brooks, 1982; Dean, 1980); mammalian cell gene mutation (Huntingdon, 1990b; Gulf Life Sciences, 1983c); chromosome aberration (Shell Development Company, 1983a, 1983c; Huntingdon, 1990c; Wilmer, 1986; Dean, 1980; Wright, 1998); transformation (Goode and Brecher, 1983a, 1983b; Shell Development Company, 1983d) and unscheduled DNA synthesis (Gulf Life Sciences, 1984a, 1984b).

### Conclusion

Based on the weight of evidence from studies with linear alpha and linear and branched internal olefins, category members are not genotoxic.

### 3.1.7 Carcinogenicity

No carcinogenicity tests have been conducted on C<sub>6</sub>-C<sub>54</sub> alpha or internal olefins. However, there are no structural alerts indicating a potential for carcinogenicity in humans.

### 3.1.8 Toxicity for Reproduction

Reproductive toxicity screening studies are available for C<sub>6</sub> and C<sub>14</sub> alpha olefins, and C<sub>6</sub> branched and C<sub>18</sub> branched and linear internal olefins. In addition, male and female reproductive organs have been examined in repeated dose studies with C<sub>6</sub> alpha olefin and C<sub>16</sub>/C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> branched and linear internal olefins (see Section 3.1.5). No evidence for reproductive effects was seen in any of these studies.

#### *Effects on Fertility*

alkenes, C<sub>6</sub> (internal, 58% branched olefin): Alkenes, C<sub>6</sub> was administered orally in a combined repeated dose/reproduction/developmental toxicity screening test (OECD 422) in which rats were exposed for a minimum of 14 days prior to mating, and continuing through lactation day 3 (Thorsrud, 2003a). Dose levels were 0, 100, 500, and 1000 mg/kg/day. There were no toxicologically meaningful differences noted in F0 bodyweights, body weight change, food consumption, gross necropsy findings, or reproductive organ weights and histopathology. There was no evidence of impaired reproductive capabilities in the F0 generation, as measured by effects on copulation and fertility, precoital intervals, gestation length, time to delivery or unusual nesting behavior. No histological changes were seen in reproductive organs of treated rats. The NOAEL for reproductive effects was >1000 mg/kg/day. The results for developmental toxicity are described below; and results from the repeated dose toxicity phase of the study are described in Section 3.1.5.

1-hexene: 1-Hexene was orally administered via gavage to male and female rats in a reproduction/developmental toxicity screening test (OECD 421) at the following doses: 0, 100, 500 and 1000 mg/kg/day in corn oil (Gingell et al., 2000). Male rats were treated for 28 days prior to

mating and for an additional 16 days (44 total days). Females were dosed for 14 days prior to mating and during mating, gestation and lactation (41-55 days). There were no effects on the following reproductive parameters: precoital intervals, gestation length, pregnancy rates, copulation and fertility indices. Absolute epididymal weights for males were statistically lower in all treated groups compared to controls and the epididymal/brain relative weights were also lower in all treated groups compared to controls (although only the low dose group was statistically significant). The biological significance of the decreased epididymal weights is uncertain because of no apparent histopathological effects in the epididymis and the lack of effect on male reproductive performance. Therefore, the NOAEL for reproductive toxicity is 1000 mg/kg/day. The results for developmental toxicity are described below. The kidney effects observed in F0 males have been described previously in section 3.1.5.

1-tetradecene: 1-Tetradecene, administered orally, was evaluated for reproductive and developmental toxicity in a combined repeated dose/reproduction/developmental toxicity screening test (OECD 422) in which male rats were exposed for 28 days prior to mating, and through mating until euthanasia for a total of 43-47 consecutive days of dosing; 12 females were dosed for 14 days prior to mating, during mating, gestation and lactation through euthanasia at lactation day 4 (42-51 consecutive days) (Daniel, 1995). A satellite group of eight females was assessed for neurotoxic analysis (see section 3.1.9). Dose levels were 0, 100, 500, and 1000 mg/kg/day. There was no evidence of impaired reproductive capabilities in the F0 generation, as measured by effects on copulation and fertility, precoital intervals, gestation length, time to delivery or unusual nesting behavior. No histological changes were seen in reproductive organs of treated rats. The NOEL for reproductive effects was >1000 mg/kg/day. The results for developmental toxicity are described below; and results from the repeated dose toxicity phase of the study are described in Section 3.1.5.

C<sub>18</sub> branched and linear internal olefin (32.5% branched): A C<sub>18</sub> branched and linear internal olefin was orally administered via gavage to male and female rats in a reproduction/developmental toxicity screening test (OECD 421) at the following doses: 0, 100, 500 and 1000 mg/kg/day in corn oil (Thorsrud, 2003b). Male rats were treated for 14 days prior to mating, during mating, and for 4 weeks following mating. Females were dosed for 14 days prior to mating and during mating, gestation and lactation (to lactation day 3). There were no toxicologically meaningful differences noted in F0 bodyweights, body weight change, food consumption, gross necropsy findings, or reproductive organ weights and histopathology. There were no effects on the following reproductive parameters: copulation and fertility, precoital intervals, gestation length, time to delivery or unusual nesting behavior. Therefore, the NOAEL for parental and reproductive toxicity is 1000 mg/kg/day. The results for developmental toxicity are described below.

### *Developmental Toxicity*

alkenes, C<sub>6</sub> (internal 58% branched): Alkenes, C<sub>6</sub>, administered orally, was evaluated in a combined repeated dose/reproduction/developmental toxicity screening test (OECD 422) in which rats were exposed for a minimum of 14 days prior to mating, and continuing through lactation day 3 at dose levels of 0, 100, 500, and 1000 mg/kg/day (Thorsrud, 2003a). There was no evidence of developmental toxicity in the F1 generation, as measured by the number of implantation sites and corpora lutea, the number of live and dead pups, number of litters with live offspring, mean litter size and male to female pup ratio, pup survival and weights, and external observations. The NOAEL for developmental effects was >1000 mg/kg/day. The results for effects on fertility are described above; and results from the repeated dose toxicity phase of the study are described in Section 3.1.5.

1-hexene: 1-Hexene was orally administered via gavage to male and female rats in a reproduction/developmental toxicity screening test (OECD 421) at dose levels of 0, 100, 500, and

1000 mg/kg/day as described above in the Effects on Fertility section (Gingell et al., 2000). There was no evidence of developmental toxicity in the F1 generation, as measured by the number of implantation sites and corpora lutea, the number of live and dead pups, number of litters with live offspring, mean litter size and male to female pup ratio, pup survival and weights, and external observations. The NOEL for developmental effects was >1000 mg/kg/day. The results for effects on fertility are described above.

1-tetradecene: 1-Tetradecene, administered orally, was evaluated for reproductive and developmental toxicity in a combined repeated dose/reproduction/developmental toxicity screening test (OECD 422) at dose levels of 0, 100, 500, and 1000 mg/kg/day, as described above in the Effects on Fertility section (Daniel, 1995). There was no evidence of developmental toxicity in the F1 generation, as measured by the number of implantation sites and corpora lutea, the number of live and dead pups, number of litters with live offspring, mean litter size and male to female pup ratio, pup survival and weights, and external observations. The NOEL for developmental effects was >1000 mg/kg/day. The results for effects on fertility are described above; and results from the repeated dose toxicity phase of the study are described in Section 3.1.5.

C<sub>18</sub> branched and linear internal olefin (32.5% branched): A C<sub>18</sub> branched and linear internal olefin was orally administered via gavage to male and female rats in a reproduction/developmental toxicity screening test (OECD 421) at dose levels of 0, 100, 500, and 1000 mg/kg/day, as described above in the Effects on Fertility section (Thorsrud, 2003b). There was no evidence of developmental toxicity in the F1 generation, as measured by the number of implantation sites and corpora lutea, the number of live and dead pups, number of litters with live offspring, mean litter size and male to female pup ratio, pup survival and weights, and external observations. The NOAEL for developmental effects was >1000 mg/kg/day. The results of the effects on fertility are described above.

### Conclusion

Based on evidence from reproduction/developmental toxicity screening tests in rats with C<sub>6</sub> and C<sub>14</sub> alpha olefins and C<sub>6</sub> and C<sub>18</sub> branched and linear internal olefins, along with the findings of no biologically significant effects on male or female reproductive organs in repeated dose toxicity studies, the Higher Olefins Category members are not considered to cause reproductive or developmental toxicity.

### 3.1.9 Neurotoxicity

Neurotoxicity was evaluated in six studies as part of other test protocols already discussed above, two performed with 1-hexene, one with alkenes, C<sub>6</sub> (internal, 58% branched), one with 1-tetradecene, one with a C<sub>16</sub>/C<sub>18</sub> internal branched and linear olefin (26% branched), and one with a C<sub>20</sub>-C<sub>24</sub> internal branched and linear olefin (>70% branched). Neurotoxicity was not observed in any of the studies. The studies utilizing 1-hexene assessed neuromuscular coordination in rats, evaluated by rotorod, which indicated no effect after oral administration for 28 days (3365 mg/kg/day) (Dotti et al., 1994) or via inhalation for 90 days (3000 ppm/10.33 mg/L) (Gingell et al., 1999). Alkenes, C<sub>6</sub> (internal branched) and 1-tetradecene were tested in combined repeated dose/reproduction/developmental toxicity screens, which evaluated a satellite group of eight female rats for motor activity, clinical pathology and functional observational battery (Thorsrud, 2003a; Daniel, 1995). Results indicated that there were no test article-related differences that would indicate neurotoxicity in rats treated orally at 1000 mg/kg/day. The study with C<sub>16</sub>/C<sub>18</sub> internal branched and linear olefin assessed neurotoxicity using a functional observation battery (Clubb, 2000). Results showed no neurotoxicity in rats treated orally at 1000 mg/kg/day for 4 weeks. When a C<sub>20</sub>-C<sub>24</sub> internal branched and linear olefins blend was tested in a 90-day rat oral repeated dose

study, which included an evaluation of motor activity and a functional observational battery, no neurobehavioral effects were seen at 1000 mg/kg/day (Brooker, 1999).

### Conclusion

Based on evidence from neurotoxicity screens included in repeated dose studies with C<sub>6</sub> and C<sub>14</sub> alpha olefins, C<sub>6</sub> internal branched olefins; and C<sub>16</sub>/C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> internal branched and linear olefins, the category members are not neurotoxic.

### 3.2 Initial Assessment for Human Health

Olefins (alkenes) ranging in carbon number from C<sub>6</sub> to C<sub>24</sub> alpha (linear) and internal (linear and branched), and C<sub>24</sub>-C<sub>54</sub> alpha (linear and branched) demonstrate low acute toxicity by the oral, inhalation and dermal routes of exposure: Rat oral LD<sub>50</sub> >5 g/kg; rat 4-hr inhalation LC<sub>50</sub> range = 110 mg/L (32,000 ppm) to 6.4 mg/L (693 ppm) for C<sub>6</sub> to C<sub>16</sub>; and rat/rabbit dermal LD<sub>50</sub> > highest doses tested (1.43-10 g/kg). Repeated dose studies, using the inhalation (C<sub>6</sub> alpha), dermal (C<sub>12</sub>-C<sub>16</sub> alpha), or oral (C<sub>6</sub> alpha and internal linear/branched; C<sub>8</sub> and C<sub>14</sub> alpha; and C<sub>16</sub>/C<sub>18</sub>, C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> internal linear/branched) routes of exposure, have shown comparable levels of low toxicity in rats. In females, alterations in body and organ weights, changes in certain clinical chemistry/hematology values, and liver effects were noted (NOELs of ≥ 100 mg/kg oral or ≥ 3.44 mg/L [1000 ppm] inhalation). In males, alterations in organ weights, changes in certain clinical chemistry/hematology values, liver effects, and kidney damage were noted (LOELs ≥ 100 mg/kg oral only). The male rat kidney damage was seen in oral studies with C<sub>6</sub>, C<sub>8</sub> and C<sub>14</sub> linear alpha olefins and C<sub>6</sub> internal branched olefins, but was not seen in studies with C<sub>16</sub>/C<sub>18</sub> or C<sub>20</sub>-C<sub>24</sub> internal linear/branched olefins. While no specific immunohistochemical staining was conducted to identify the hyaline droplets associated with the observed kidney effects, their morphology and occurrence only in male rats suggest that they are probably related to alpha<sub>2μ</sub>-globulin nephropathy, a male rat specific effect that is not considered relevant to human health. The noted liver effects were seen in oral studies with C<sub>14</sub> alpha olefins (minimal-to-mild hepatocyte cytoplasmic vacuolation with increased liver weight in males and females) and with C<sub>20</sub>-C<sub>24</sub> internal olefins (minimal centrilobular hepatocyte hypertrophy with increased liver weight in females only). No effects were present in the study with C<sub>20</sub>-C<sub>24</sub> internal olefins following a 4-week recovery period, indicating reversibility of the observed effects. These liver effects seen only with the larger molecules may be indirect effects of an intensified liver burden, rather than a direct toxic effect of the olefin. Based on evidence from neurotoxicity screens included in repeated dose studies with C<sub>6</sub> and C<sub>14</sub> alpha olefins and with C<sub>6</sub>, C<sub>16</sub>/C<sub>18</sub> and C<sub>20</sub>-C<sub>24</sub> internal linear/branched olefins, the category members are not neurotoxic. Based on evidence from reproductive/developmental toxicity screens in rats with C<sub>6</sub> and C<sub>14</sub> alpha olefins and C<sub>6</sub> and C<sub>18</sub> linear/branched internal olefins, along with the findings of no biologically significant effects on male or female reproductive organs in repeated dose toxicity studies, the category members are not expected to cause reproductive or developmental toxicity. Based on the weight of evidence from studies with alpha and internal olefins, category members are not genotoxic. No carcinogenicity tests have been conducted on C<sub>6</sub>-C<sub>54</sub> alpha or internal olefins; however, there are no structural alerts indicating a potential for carcinogenicity in humans. These materials are not eye irritants or skin sensitizers. Prolonged exposure of the skin for many hours may cause skin irritation. The weight of evidence indicates alpha and internal olefins with carbon numbers between C<sub>6</sub> and C<sub>54</sub> have a similar and low level of mammalian toxicity, and the toxicity profile is not affected by changes in the location of the double bond or the addition of branching to the structure. Thus, the data available for the C<sub>6</sub>-C<sub>54</sub> alkenes are adequate to characterize the human health hazards of substances included in the Higher Olefins Category and justify the category designation. The data indicate a low hazard potential for human health for members of the Higher

Olefins Category, which is consistent with the conclusion reached at SIAM 11 for the Alpha Olefins Category.

## 4 HAZARDS TO THE ENVIRONMENT

### 4.1 Aquatic Effects

Products in this category are expected to cause a relatively narrow range of toxicity to freshwater fish, invertebrates, and algae. This assessment is based on existing data for products that can be used to read across to this category and results of computer modelling using ECOSAR for selected chemical components of product streams in this category [ECOSAR is an aquatic toxicity modelling program and is a subroutine contained in EPIWIN (EPIWIN, 1999a,b; 2000a,b)]. The relatively narrow range of toxicity for the lower molecular weight members of the category is not unexpected because:

- Constituent chemicals of products in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis and whose potencies are equivalent.
- Although the double bond location is different for alpha and internal olefins, for same carbon number olefins, the aquatic toxicity of the two types of olefins are anticipated to be similar.

The toxic mechanism of short-term toxicity for these types of chemicals is disruption of biological membrane function (van Wezel and Opperhuizen, 1995), and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen et al., 2000). The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between 4-5 mmol/kg fish (wet weight) (McCarty and Mackay, 1993; McCarty et al., 1991), and supports the assessment that these chemicals have equal potencies within the range of solubility that results in toxicity. When normalized to lipid content, the CBR is approximately 50  $\mu\text{mol}$  of hydrocarbon/g of lipid for most organisms (DiToro et al., 2000).

The members of the Higher Olefins Category include alpha and internal olefins. Computer modelling suggests that aquatic toxicity does not differ with bond location, alpha compared to internal. The data shown in Tables 10 and 11 illustrate this point. EPIWIN (EPIWIN, 1999b, 2000b) was used to estimate the water solubility and octanol/water partitioning coefficient ( $K_{ow}$ ) values. The log  $K_{ow}$  was then used in the U.S. EPA's ECOSAR computer program (EPIWIN, 1999b, 2000b) to estimate toxicity to fish, *Daphnia*, and alga.

Table 10 compares calculated acute toxicity values of  $C_6$ - $C_{10}$  internal olefins for a fish, *Daphnia*, and alga. Calculated water solubility and log  $K_{ow}$  values are also presented for these chemicals. The data show that toxicity increases with increasing carbon number, which is consistent with increasing  $K_{ow}$  values. In comparison, water solubility for these olefins decreases as carbon number increases. Toxicity values for  $C_{12}$ - $C_{54}$  olefins are not included because olefins in this molecular weight range will not cause acute toxicity for the endpoints listed in Table 10. The lack of acute toxicity is due to water solubility limitations for chemicals in this range of carbon numbers. In other words, higher molecular weight olefins will not be in solution at concentrations that will result in a CBR within the range that would produce mortality.

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

**Table 10** Calculated aquatic toxicity, water solubility and log Kow values for selected C<sub>6</sub> to C<sub>10</sub> internal olefins<sup>a</sup>

Chemical	CAS #	Fish 96h LC50 (mg/L)	Daphnid 48h LC50 (mg/L)	Green Algae 96h EC50 (mg/L)	Water Solubility (calculated) (mg/L) <sup>b</sup>	Log Kow (calculated)
Hexene <sup>c</sup>	25264-93-1	6.16	7.10	4.72	30.32	3.07
Heptene <sup>d</sup>	25339-56-4	2.09	2.51	1.73	9.27	3.64
Octene <sup>d</sup>	25377-83-7	0.83	1.03	0.73	3.35	4.13
Nonene <sup>c</sup>	27215-95-8	0.38	0.48	0.35	1.41	4.55
Decene <sup>d</sup>	25339-53-1	0.12	0.16	0.12	0.41	5.12

<sup>a</sup> EPIWIN (EPIWIN, 2000b) was used to estimate the water solubility and octanol/water partitioning coefficient (Kow) values. The log Kow was then used in the U.S. EPA's ECOSAR computer program to estimate toxicity to fish, *Daphnia*, and alga.

<sup>b</sup> Value shown is value used by EPIWIN for ECOSAR calculation.

<sup>c</sup> EPIWIN used structure with double bond between second and third carbons.

<sup>d</sup> EPIWIN used alpha structure.

Table 11 compares a second set of calculated toxicity values between alpha and internal olefins. These data show that similar toxicity is expected for a carbon number regardless of bond location. A comparison of toxicity values for 1-, 2-, and 3- hexene for a fish, *Daphnia*, and alga show similar toxicity within each individual organism. This similarity in toxicity for each carbon number is consistent through 1- and 5-decene. As seen with the data presented in Table 10, toxicity increases as carbon chain length increases.

**Table 11** Calculated aquatic toxicity, water solubility, and log Kow values for selected C<sub>6</sub> to C<sub>10</sub> alpha and internal olefins<sup>a</sup>

Chemical	CAS #	Fish 96h LC50 (mg/L)	Daphnid 48h LC50 (mg/L)	Green Alga 96h EC50 (mg/L)	Water Solubility (calculated) (mg/L) <sup>b</sup>	Log Kow (calculated)
1-Hexene	592-41-6	5.18	6.01	4.01	25.13	3.15
t-2-Hexene	4050-45-7	6.16	7.10	4.72	30.32	3.07
t-3-Hexene	13269-52-8	6.16	7.10	4.72	30.32	3.07
1-Heptene	592-76-7	2.09	2.51	1.73	9.27	3.64
t-2-Heptene	14686-13-6	2.49	2.97	2.03	11.19	3.56
t-3-Heptene	14686-14-7	2.49	2.97	2.03	11.19	3.56
1-Octene	111-66-0	0.83	1.03	0.73	3.35	4.13
t-2-Octene	13389-42-9	0.96	1.19	0.84	3.95	4.06
3-Octene	14919-01-8	0.96	1.19	0.84	3.95	4.06
t-4-Octene	14850-23-8	0.96	1.19	0.84	3.95	4.06
1-Decene	872-05-9	0.12	0.16	0.12	0.41	5.12

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

t-5-Decene	7433-56-9	0.14	0.19	0.14	0.50	5.04
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<sup>a</sup> EPIWIN (EPIWIN, 2000b) was used to estimate the water solubility and octanol/water partitioning coefficient (K<sub>ow</sub>) values. Default values were used for calculations. The log K<sub>ow</sub> was then used in the U.S. EPA's ECOSAR computer program to estimate toxicity to fish, *Daphnia*, and alga.

<sup>b</sup> Value shown is the default calculated water solubility value that ECOSAR used for the toxicity calculations.

Acute Aquatic Toxicity Test Results

For acute aquatic toxicity, the existing data (Table 12) indicate that through the C<sub>10</sub> olefins, acute toxicity can be observed (C<sub>6</sub>: EC/LC<sub>50</sub> range of 1-10 mg/L; C<sub>7</sub>-C<sub>10</sub>: EC/LC<sub>50</sub> range of 0.1-1.0 mg/L), and that toxicity increases with increasing carbon number within that range, which is consistent with increasing K<sub>ow</sub> values (3.07 – 5.12). Product solubility during toxicity testing is critical to understanding both observations and estimates of effects. Solubility is within the range of observed acute toxicity. For an internal decene stream (CAS No. 25339-53-1), the acute toxicity to fish was observed to be 0.12 mg/L and the corresponding estimated solubility using ECOSAR suite (EPIWIN, 2000b) is 0.41 mg/L. The effects seen in algae, *Daphnia*, and fish are approximately equal at water solubility. However, since that value is the LC50, there were concentrations above the LC50 of 0.12 mg/L that may not have been in solution. Above a chain length of 10, toxicity is not observed within the limits of solubility. The results for tetradecene and higher carbon numbers indicating LL0/EL0 > 1000 mg/L only show that there was no toxicity at any exposure concentration. The solubility was too low to have resulted in toxicity. Therefore, meaningful acute toxicity data can be identified only at or below C<sub>10</sub> where solubility is high enough to allow the acute effects to be expressed.

Determining the aquatic toxicity of products that have relatively low water solubility and higher vapour pressure, like those in this category, can be difficult because they tend not to remain in solution. These data show that the measured and calculated values are in good agreement through octene, and they also support that the test methods used procedures that were able to maintain exposures. These data are believed to form a sufficiently robust dataset to fully characterize the acute aquatic toxicity endpoints in the US EPA HPV Chemical Challenge Program.

Table 13 Algae toxicity and invertebrate and fish acute toxicity of C<sub>6</sub>-C<sub>24</sub> alkenes<sup>a</sup>

Chemical <sup>b</sup>	Acute Toxicity to Fish (Rainbow trout unless otherwise specified) (mg/L)	Acute Toxicity to Invertebrates ( <i>Daphnia</i> ) (mg/L)	Acute Toxicity to Plants (Algae) (mg/L)
Hexene (CAS# 25264-93-1)	NDA	NDA	NDA
Alkenes, C6 (internal branched stream) (CAS# 68526-52-3)	96-hr LC50 = 6.6 (measured) 96-hr LL50 = 12.8 (nominal) 96-hr NOEC = 2.9 (measured) Mortality, semi-static; no headspace. WAF <sup>d</sup>	48-hr EC50 = 4.4 (measured) 48-hr EL50 = 20 (nominal) Static, sealed vessel conditions with minimal headspace	96-hr EC50 (cell density) = 4.6 96-hr NOEC (cell density) = 1.8 96-hr E <sub>50</sub> (biomass) = 4.5 96-hr NOEC (biomass) = 0.23 96-hr E <sub>50</sub> (growth rate) >5.5 96-hr NOEC (growth rate) = 1.8

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical <sup>b</sup>	Acute Toxicity to Fish (Rainbow trout unless otherwise specified) (mg/L)	Acute Toxicity to Invertebrates (Daphnia) (mg/L)	Acute Toxicity to Plants (Algae) (mg/L)
			(measured) Static; WAF sealed vessel conditions with no headspace
Neohexene (CAS# 558-37-2)	NDA	NDA	NDA
1-hexene (CAS# 592-41-6)	24,48,72,96-hr LC50 = 9.7, 5.6, 5.6 and 5.6 (measured) Semi-static, minimal headspace to prevent losses through evaporation	48-hr EL50 = 30 (estimated); NOEC = 10 (nominal) Static, stoppered flask	96-hr EC50 > solubility 96-hr EL0 > 22 (22 mg/L was the highest nominal concentration tested that was below the water solubility) Static; endpoint was biomass; no attempt to prevent evaporation; no reduction in cell numbers at 1000 mg/L (nominal)
Heptene (CAS# 25339-56-4)	NDA	NDA	NDA
Alkenes, C6-8, C7 rich (internal stream) (CAS# 68526-53-4)	NDA	NDA	NDA
Octene (CAS# 25377-83-7)	NDA	NDA	NDA
Alkenes, C7-9, C8 rich (internal stream) (CAS# 68526-54-5)	96-hr LC50 = 0.87 (measured) 96-hr LL50 = 8.9 (nominal) 96-hr NOEC = 0.4 (measured) Mortality; semi-static, no headspace, WAF	NDA	NDA
2-Octene (trans) (CAS# 111-67-1)	Zebra fish ( <i>Brachiodanio rerio</i> ) 96-hr LL50 = 7.5 (nominal) 96-hr NOEC = 3.2 (nominal) Semi-static, stirred 4 hr before adding fish, glass-stoppered flask	48-hr EL50 > 3.2 < 10 (nominal) (est. to be about 6) 48-hr NOEC = 3.2 (nominal) Static, stirred 4 hr before adding test animals; tested in glass-stoppered flask	NDA
1-Octene (CAS# 111-66-0)	Zebra fish ( <i>Brachiodanio rerio</i> ) 24-96-hr LL50 > 3.2 < 10 (nominal) (est. to be about 6) 96-hr NOEC = 3.2 (nominal) Semi-static, stirred 4 hr before adding fish, glass-stoppered flask	48-hr EL50 > 3.2 < 10 (nominal) (est. to be about 6) 48-hr NOEC = 3.2 (nominal) Static, stirred 4 hr before adding test animals; tested in glass-stoppered flask	NDA

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical <sup>b</sup>	Acute Toxicity to Fish (Rainbow trout unless otherwise specified) (mg/L)	Acute Toxicity to Invertebrates (Daphnia) (mg/L)	Acute Toxicity to Plants (Algae) (mg/L)
Nonene (CAS# 27215-95-8)	NDA	NDA	NDA
1-Nonene (CAS# 124-11-8)	Zebra fish ( <i>Brachiodanio rerio</i> ) 48-hr LL50 > 3.2 < 10 (nominal) (est. to be about 6) 96-hr LL50 < 3.2 (nominal) Semi-static, stirred 4 hr before adding fish, glass-stoppered flask	48-hr EL50 < 3.2 (nominal) (est. to be about 2) Static, stirred 4 hr before adding test animals; tested in glass-stoppered flask	NDA
Alkenes, C8-10, C9 rich (internal stream) (CAS# 68526-55-6)	NDA	NDA	NDA
Alkenes, C9-11, C10 rich (internal stream) (CAS# 68526-56-7)	96-hr LC50 = 0.12 (measured) 96-hr NOEC = 0.06 (measured) 96-hr LL50 = 4.8 (nominal) Mortality, semi-static; no headspace. WAF; mortality at ≥ 0.08 mg/L	NDA	NDA
Alkenes, C10-12, C11 rich (internal stream) (CAS# 68526-53-4)	NDA	NDA	NDA
C10,12 olefin rich hydrocarbons (CAS# 68514-32-9)	NDA	NDA	NDA
Alkenes, C10-13 (CAS# 85535-87-1) (Studies conducted with C10-13 internal olefin blends having composition different from the current product)	96-hr LC50 > solubility 96-hr LL0 = 1000 (nominal) Semi-static, vessels not sealed, solution aerated. Concentrations utilized in testing were greater than the water solubility; 2 studies; no mortality in 1 study and 1/10 fish died in the other study	48-hr EL50 = 0.74 (nominal) Static, vessels not sealed, no headspace; no dissolved test substance observed at the highest dose (5 mg/L)	NDA
Alkenes, C10-16 alpha (CAS# 68855- 58-3)	NDA	NDA	NDA
Alkenes, C10-16 (CAS# 68991-52-6)	NDA	NDA	NDA
Dodecene (CAS# 25378-22-7)	NDA	NDA	NDA
Alkenes, C11-13, C12 rich (internal branched stream) (CAS# 68526-58-9)	96-hr EC50 > solubility 96-hr LL0 = 86.0 (nominal, estimated to be < 0.20 [lowest analyzed standard])	NDA	NDA

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical <sup>b</sup>	Acute Toxicity to Fish (Rainbow trout unless otherwise specified) (mg/L)	Acute Toxicity to Invertebrates (Daphnia) (mg/L)	Acute Toxicity to Plants (Algae) (mg/L)
	Mortality, semi-static; no headspace; WAF; no mortality		
Heavy polymerization naphtha (petroleum) (CAS # 68783-10-8)	NDA	NDA	NDA
1-Tridecene (CAS#2437-56-1)	NDA	NDA	NDA
C12-14 olefin rich hydrocarbons (CAS# 68514-33-0)	NDA	NDA	NDA
1-Tetradecene 99% (CAS# 1120-36-1)	96-hr LC50 > solubility Actual concentration negligible. 96-hr LLO = 1000 (nominal) Mortality; semi-static test; WAF; concentration utilized in testing greater than water solubility; TOC <sup>c</sup> analysis at 0 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L	48-hr EC50 > solubility. Actual concentration negligible. 24-hr ELO and 48-hr ELO = 1000 (nominal) Immobility; semi-static test; WAF; concentration utilized in testing greater than water solubility; TOC analysis at 0 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L	96-hr EC50 > solubility. Actual concentration negligible. 72- 96 hr ELO = 1000 (nominal) Growth; static test; WAF; concentration utilized in testing greater than water solubility; no toxicity seen at 1000 mg/L
Alkenes, C14-18 alpha (CAS#68855- 59-4)	NDA	NDA	NDA
Alkenes, C14-20 alpha (CAS#68855- 60-7)	NDA	NDA	NDA
Alkenes, C15-18 (CAS#93762-80-2)	NDA	NDA	NDA
1-Hexadecene (CAS# 629-73-2)	96-hr LC50 > solubility Actual concentration negligible. 96-hr LLO = 1000 (nominal) Mortality; semi-static test; WAF; concentrations utilized in testing greater than water solubility; TOC analysis at 0 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L	NDA	72-hr EC50 > solubility 24-48-hr EC50 > solubility Actual concentration negligible. 72-hr ELO = 1000 (nominal) Growth; static test; WAF; concentration utilized in testing greater than water solubility; TOC analysis at 0 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical <sup>b</sup>	Acute Toxicity to Fish (Rainbow trout unless otherwise specified) (mg/L)	Acute Toxicity to Invertebrates (Daphnia) (mg/L)	Acute Toxicity to Plants (Algae) (mg/L)
1-Octadecene (CAS# 112-88-9)	96-hr LC50 > solubility 96-hr LLO = 1000 (nominal) Mortality; semi-static test; concentrations utilized in testing greater than solubility; no toxicity seen at 1000 mg/L	24-hr and 48-hr EC50 > solubility 24-hr and 48-hr EL50 >1000 (nominal) Immobility; static test; concentrations utilized in testing greater than water solubility; <4% immobilized during 48-hr exposure to 1000 mg/L (nominal)	96-hr EC50 > solubility 96-hr ELO = 1000 (nominal) Growth; static test; concentrations utilized in testing greater than solubility; no toxicity seen at 1000 mg/L
C16/C18 internal linear and branched blend (50/50) (CAS# 26952-14-7)	Turbot ( <i>Scophthalmus maximus</i> ) 96-hr LC50 > solubility 96-hr LLO = 10,000 (nominal) Mortality; semi-static test; concentrations utilized in testing greater than water solubility; no toxicity seen at 10,000 mg/L	NDA	NDA
1-Eicosene (CAS#3452-07-1)	NDA	NDA	NDA
1-Docosene (CAS#1599-67-3)	NDA	NDA	NDA
1-Tetracosene (CAS#10192-32-2)	NDA	NDA	NDA
C20-24 linear alpha olefin blend (CAS# 93934-10-8)	96-hr LC50 > solubility Actual concentrations negligible. 96-hr LLO = 1000 (nominal) Mortality; semi-static test; WAF; concentrations utilized in testing greater than solubility; TOC analysis at 0 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L	NDA	72-hr EC50 > solubility Actual concentration negligible 72-hr ELO = 1000 (nominal) Growth rate; area under the curve; static test; WAF concentrations utilized in testing greater than solubility; TOC analysis at 0 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L
α-Olefin fraction C24-28 cut (CAS# 93924-11-9)	NDA	NDA	NDA

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical <sup>b</sup>	Acute Toxicity to Fish (Rainbow trout unless otherwise specified) (mg/L)	Acute Toxicity to Invertebrates ( <i>Daphnia</i> ) (mg/L)	Acute Toxicity to Plants (Algae) (mg/L)
C20-24 internal linear and branched blend (C20 CAS# 182636- 03-9; C22 CAS# 182636-04-0; C24 CAS# 182636-05-1)	96-hr LC50 > solubility Actual concentrations negligible. 96-hr LL0 = 1000 (nominal) Mortality; semi-static test; WAF; concentrations utilized in testing greater than solubility; TOC analysis at 0 hr and at end of 1 <sup>st</sup> 24 hr of testing demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L	48-hr EC50 > solubility Actual concentrations negligible. 48-hr EL0 = 1000 (nominal) Immobility; static test; WAF; concentrations utilized in testing greater than solubility; TOC analysis at 0 and 48 hr demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L	96-hr EC50 > solubility Actual concentrations negligible. 96-hr EL0 = 1000 (nominal) Growth; static test; WAF; concentrations utilized in testing greater than solubility; TOC analysis at 0 hr and at end of test demonstrated that values for exposure media were no greater than control value; no toxicity seen at 1000 mg/L
Alkene, C24-54 branched and linear, alpha (CAS# 131459-42-2)	NDA	NDA	NDA

<sup>a</sup> Study details and references are found in the robust summaries in the dossiers.

<sup>b</sup> Higher Olefins Category members are shaded.

<sup>c</sup> NDA: No reliable data available

<sup>d</sup> WAF: Water accommodated fractions used due to the low water solubility of the test material.

<sup>e</sup> TOC: Total Organic Carbon

Chronic Toxicity Test Results

No existing chronic toxicity data were found for C<sub>6</sub>- C<sub>54</sub> alpha or internal olefins. Initially, a chronic daphnia toxicity study (OECD 211) using 1-dodecene was attempted. However, due to analytical limitations and the lab's inability to detect the material in solution, the lab was unable to generate a reproducible dose response. Based on inability to test the C<sub>12</sub> olefin, and on the acute toxicity results shown in Table 12 and a log Kow value >4.2, a C<sub>10</sub> alpha olefin was selected for testing in chronic aquatic invertebrates (*Daphnia*), to clarify the chronic toxicity of this category. The 1-decene *Daphnia magna* 21 day EC<sub>10</sub> was 20.0 µg/L and the EC<sub>50</sub> was 28.1 µg/L (ExxonMobil, 2004). Reproduction and growth were more sensitive than survival, resulting in a NOEC of 19.4 µg/L and a LOEC of 28.7 µg/L. The maximum water solubility of 1-decene under the conditions used to generate the stock solution was approximately 210 µg/L.

The chronic toxicity values estimated for representative C<sub>6</sub> – C<sub>13</sub> alpha and/or internal olefins using the computer program ECOSAR (EPIWIN, 2000b) are generally consistent with the experimental value for 1-decene (see Table 13). Chronic toxicity is not expected for C<sub>14</sub> and higher molecular weight alpha or internal olefins, whose water solubility limits are less than the NOEC for 1-decene.

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

**Table 15** Predicted chronic toxicity results for representative C<sub>6</sub> – C<sub>13</sub> members or components of members of the Higher Olefins Category <sup>a</sup>

Chemical	CAS#	Fish 30-day ChV (µg/L)	Daphnia 16-day EC50 (µg/L)	Algae 96-hr ChV (µg/L)
Hexene/Alkenes, C6/ Neohexene	25264-93-1/ 68526-52-3/ 558-37-2	942/ 803/1001	582/509/ 611	876/780/ 916
Heptene/ Alkenes, C6-8, C7 rich	25339-56-4/ 68526-53-4	351	264	445
Octene/1-octene/ Alkenes, C7-9, C8 rich	25377-83-7/ 111-66-0/ 68526-54-5	150	134	249
Nonene/ Alkenes, C8-10, C9 rich	27215-95-8/ 68526-55-6	73/ 63	75/ 67	152/ 137
Decene/ 1-decene/ Alkenes, C9-11, C10 rich	25339-53-1/ 872-05-9/ 68526-56-7	26/ 26/ 59	32/ 32/ 64	73/ 73/ 133
Undecene/ Alkenes, C10- 12, C11 rich	28761-27-5/ 68526-57-8	13/ 11	18/ 16	44/ 39
Dodecene/ 1-dodecene / Alkenes C11-13, C12 rich	25378-22-7/ 112-41-4/ 68526-58-9	4	8	21
Tridecene/ 1-tridecene	25377-82-6/ 2437-56-1	2	4	11

<sup>a</sup> EPIWIN (EPIWIN, 2000b) was used to estimate the octanol/water partitioning coefficient (Kow) values. The log Kow was then used in the U.S. EPA's ECOSAR computer program to estimate chronic toxicity values (ChV) for fish and algae and a 16-day EC50 value for Daphnia. CAS#s were used for input into EPIWIN. EPIWIN used alpha structures for all except hexene, nonene, undecene and alkenes, C9-11, C10 rich.

Toxicity to Microorganisms

Available data for C<sub>6</sub>, C<sub>8</sub>, C<sub>10</sub>, C<sub>14</sub> and C<sub>18</sub> alpha olefins and C<sub>20</sub>-C<sub>24</sub> internal olefins (see Table 14) suggest that the members of the Higher Olefins Category do not cause toxicity to microorganisms at saturation levels.

**Table 16** Summary of toxicity to microorganisms<sup>a</sup>

Chemical	Species	Method	Result
1-hexene	(1) <i>Pseudomonas fluorescens</i> (2)13 marine bacteria	(1) 79/931/EEC, Annex V. According to <i>Degradability,</i> <i>Ecotoxicity, and</i> <i>Bioaccumulation</i> , TNO, Delft, The Netherlands, 1977  (2) Acute static bioassay	(1)Maximum inhibition was 24% at 1000 mg/L (2)Toxic effect [log EC10 (mol/L) = -0.49]; log EC50 > saturation level
1-octene	13 marine bacteria	Acute static bioassay	EC50 > saturation level
1-decene	13 marine bacteria	Acute static bioassay	EC50 > saturation level

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical	Species	Method	Result
1-tetradecene	(1) <i>Pseudomonas fluorescens</i> (2)13 marine bacteria (3) <i>Candida sp.</i> and <i>Saccharomyces carlsbergensis</i>	(1)comparable to guideline study (2)Acute static bioassay (3)growth inhibition	(1)EC50 >1000 mg/L (2)EC50 > saturation level (3)Good growth w/glucose; w/out glucose: good growth in <i>Candida</i> ; no growth in <i>Saccharomyces</i>
1-octadecene	<i>Pseudomonas fluorescens</i>	79/931/EEC, Annex V. According to <i>Degradability, Ecotoxicity, and Bioaccumulation</i> , TNO, Delft, The Netherlands, 1977	EC50 > 1000 mg/L
C20-24 alkenes, internal branched and linear	Sewage sludge micro-organisms	OECD 209	EC50 > 1000 mg/L at 30 min and 3 hr (did not inhibit the respiration rate of activated sewage sludge)

<sup>a</sup> Study details and references are found in the robust summaries in the dossiers.

### 4.2 Terrestrial Effects

There were no terrestrial toxicity studies found for the members of the Higher Olefins Category or structural analogues.

Based on Level III fugacity modelling, the estimated partitioning of these chemicals indicates that there is a potential (increasing with chain length) to partition to the sediment and soil compartments, if released to the environment.

### 4.3 Other Environmental Effects

No data available.

### 4.4 Initial Assessment for the Environment

The potential for exposure of aquatic organisms to members of the Higher Olefins Category will be influenced by their physico-chemical properties. The predicted or measured water solubilities of these olefins range from 50 mg/L at 20°C for hexene to 0.00015 mg/L at 25°C for 1-octadecene, and to 6.33 [E-23] mg/L at 25°C for C<sub>54</sub> alpha olefin, which suggests there is a lower potential for the larger olefins to be bioavailable to aquatic organisms due to their low solubilities. Their vapor pressures range from 230.6 hPa at 25°C for hexene to 0.00009 hPa at 25°C for 1-octadecene, and to 1.13 [E-16] hPa at 25°C for C<sub>54</sub> alpha olefin, which suggests the shorter chain olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for long periods of time; while the longer chain olefins will tend to partition primarily to water, soil or sediment, depending on water solubility and sorption behavior. The predicted soil adsorption coefficients (K<sub>oc</sub>) range from 149 for C<sub>6</sub> to 230,800 for C<sub>18</sub>, and to 1.0 [E10] for C<sub>54</sub>, indicating increasing partitioning to soil/sediment with increasing carbon number. Level I fugacity modelling predicts that the C<sub>6</sub>-C<sub>13</sub> olefins would partition primarily to air, while the C<sub>16</sub> and longer chain olefins would partition primarily to soil. Results of Level III fugacity modelling suggest that the C<sub>6</sub> – C<sub>8</sub> category members will partition primarily to the water compartment; and, as the chain length increases beyond C<sub>10</sub>, soil and sediment become the primary compartments. These chemicals have a very low potential to hydrolyze and do not photodegrade directly. However, in the air, all members of the category are subject to atmospheric oxidation from hydroxyl radical attack, with calculated

degradation half-lives of 1.8 to 4.8 hours. C<sub>6</sub> – C<sub>30</sub> olefins have been shown to degrade to an extent of approximately 8-92% in standard 28-day biodegradation tests. These results were not clearly correlated with carbon number or any other identifiable parameter; however, the weight of evidence shows that the members of the Higher Olefins Category have potential for degradation in the environment. Volatilization from water is predicted to occur rapidly (hours to days), with Henry's Law Constants (bond method) ranging from 0.423 (C<sub>6</sub>) to 10.7 (C<sub>18</sub>), and to 2.89 [E5] (C<sub>54</sub>) atm<sup>3</sup>/mol. Consideration of these degradation processes supports the assessment that these substances will degrade relatively rapidly in the environment and not persist. Based on calculated bioconcentration factors, the C<sub>6</sub>, C<sub>7</sub>, and C<sub>16</sub> and longer chain length category members are not expected to bioaccumulate (BCF: C<sub>6</sub> = 44-46, C<sub>7</sub> = 236, C<sub>16</sub> = 71-92 and  $\geq$  C<sub>18</sub> = 3.2-4.6). Although the C<sub>8</sub> – C<sub>15</sub> olefins have BCFs ranging from 313 to 2030, and K<sub>ow</sub> values ranging from 4.13 to 7.49, and thus are considered to have the potential for bioaccumulation, their physico-chemical properties and fate indicate that there would be limited environmental exposure because of volatility, biodegradability and limited solubility. Data indicate that acute aquatic toxicity can be observed for C<sub>6</sub> through the C<sub>10</sub> olefins (C<sub>6</sub>: EC/LC50 range of 1-10 mg/L; C<sub>7</sub>-C<sub>10</sub>: EC/LC50 range of 0.1-1.0 mg/L), and that toxicity increases with increasing carbon number within that range, which is consistent with increasing K<sub>ow</sub> values (3.07 – 5.12). Above a chain length of 10, toxicity is not observed within the limits of solubility. However, data indicate that chronic aquatic toxicity can be observed in the C<sub>10</sub> olefins (EC10 = 20.0  $\mu$ g/L, EC50 = 28.1  $\mu$ g/L, NOEC = 19.04  $\mu$ g/L). Data also suggest that aquatic toxicity does not differ with bond location or presence of branching. Sufficient data are available to characterize the environmental hazards of members of the Higher Olefins Category.

## 5 RECOMMENDATIONS

The chemicals in the Higher Olefins Category are currently of low priority for further work.

These chemicals possess properties indicating hazards to human health (reversible mild skin and eye irritation; mild respiratory tract irritation to the lower chain length members) and the environment (acute aquatic toxicity for the C<sub>6</sub>-C<sub>10</sub> category members and chronic aquatic toxicity for C<sub>10</sub>). Based on available exposure data for the U.S (five manufacturing sites) and relating to use pattern in the U.S. (primarily as industrial intermediates in closed systems) this category is a low priority for further work.

Category Analysis: A large amount of data for mammalian and environmental endpoints on members of the Higher Olefins Category and analogous substances (C<sub>6</sub>-C<sub>54</sub>) alpha and internal olefins indicate an increasing or decreasing trend or pattern, irrespective of location of double bond, or presence or absence of branching, from the shortest to the longest olefin in the database for various physico-chemical properties and ecotoxicity (using a mixture of experimental data and estimation techniques), whereas there appears to be no critical difference across category members for biodegradation and health endpoints. Thus, the use of data from structural analogues for read-across to members of the category is appropriate, and designation of the Higher Olefins as a category is justified.

## 6 REFERENCES

ACGIH (American Conference of Governmental Industrial Hygienists) (2003). 2003 TLVs® and BEIs® Based on the Documentation of the Threshold Limit Values for Chemical Substances and Physical Agents & Biological Exposure Indices. ACGIH.

Albro PW and Fishbein L (1970). Absorption of aliphatic hydrocarbons by rats. *Biochim. Biophys. Acta* 219:437-446.

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

---

American Chemistry Council, Higher Olefins Panel (2002). Personal communications.

Baetcke KP, Hard GC, Rodgers SI, and McGaughy RE (1990). Report of the EPA Peer Review Workshop on Alpha 2 $\mu$ -Globulin Association with Renal Toxicity and Neoplasia in the Male Rat. U.S. Environmental Protection Agency, Washington, D.C.

Brooker AJ (1999). Toxicity study by oral gavage administration to CD rats for 13 weeks followed by a 4-week recovery period, Project Nos. CHR/052 and CHR/053. Conducted for Chevron Research and Technology Company (unpublished report).

Brooks, T.M. (1982) Toxicity of detergents/higher olefins: In vitro genotoxicity studies on Shop products (olefins C11 – C12 and C13 – C14, olefin HE bleed and olefin intermediate recycle). Sittingbourne, Shell Research Limited, SBGR.81.325 (unpublished report).

Brooks, TM, Clare, MG, Wiggins, DE (1983) Toxicity studies with detergents: Genotoxicity studies with Olefin 103 PQ/11 (Cracked Urea Wax Olefin). Shell Research Limited, SBGR.83.299 (unpublished report).

Burghardtova, K. , B. Horvathova and M. Valachova (1984) Testing of some 1-alkenes by the method of Ames. Biologia (Bratislava), vol. 39(11):1121-1125 (in Czech.) (unpublished report).

Cavender, F (1998). Aliphatic Hydrocarbons. In: Patty's Industrial Hygiene and Toxicology. CD-ROM. Vol. 2B, Chapter 19. Edited by Clayton GD, Clayton FE, Cralley LJ, Cralley LV, Harris RL and Bus JS. John Wiley & Sons, Inc., 1249.

Clubb S (2000). AmoDrill 1000 4-week toxicity study including neurotoxicity screening in rats with administration by gavage. Inveresk Project Number 454729. Inveresk Report Number 17561. Inveresk Research Tranent EH33 2NE. Scotland. Sponsor Amoco Corporation (unpublished report).

Daniel EM (1995). Combined repeated dose toxicity study/reproduction/developmental toxicity screening test in rats with 1-tetradecene. Conducted by Springborn Laboratories, Inc., Spencerville, Ohio, Study No. 3325.2 for the Chemical Manufacturers Association, Alpha Olefins Panel.

Dean BJ. Shell Chemicals Europe Ltd. (1980). Toxicity Studies with Detergent Intermediates: In Vitro Genotoxicity Studies with SHOP Process Intermediates. Shell Toxicology Laboratory (Tunstall). Shell Report # TLGR.80.074 (unpublished report).

De Rooij JF, Woldhuis J, Kemp G, Kollard H (1993). Analysis of hydrocarbon residues in rat livers. Appendix to CONCAWE Report No. 93/56, White oil and waxes – summary of 90-day studies. 1993. CONCAWE, Brussels.

Di Toro DM, McGrath JA, and Hansen DH (2000). Technical basis for narcotic chemicals and polycyclic aromatic hydrocarbon criteria. I. Water and Tissue. Environmental Toxicology and Chemistry **19**, 1951-1970.

Dotti A, Duback-Powell JR, Biderman K, and Weber K (1994). 4-Week oral toxicity (gavage) study with 1-hexene in the rat. RCC Project 332695. Cited in HEDSET.

Durward R (1998) C20-24 Alkenes, Branched and Linear: Micronucleus Test in the Mouse, SafePharm Laboratories Limited Project No. 703-121. Conducted for Chevron Research and Technology Company (unpublished report).

Eide I, Hagerman R, Zahlens K, Tareke E, Tornquist M, Kumar R, Vodicka P and Hemminki K (1995). Uptake, distribution, and formation of hemoglobin and DNA adducts after inhalation of C2-C8 1-alkenes [olefins] in the rat. Carcinogenesis. **16**, 1603 - 1609.

EPIWIN (1999a). Estimation Program Interface for Windows, version unknown (used by EPA for calculations presented in the SIAR for the C6-C14 alpha olefins approved at SIAM 11). Syracuse Research Corporation, Syracuse, NY, USA.

EPIWIN (1999b). Estimation Program Interface for Windows, version 3.02. Syracuse Research Corporation, Syracuse, NY, USA.

EPIWIN (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY, USA.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

Exxon Biomedical Sciences, Inc. (1991a). Alkenes, C6: Microbial Mutagenesis in *Salmonella*: Mammalian Microsome Plate Incorporation Assay. Conducted by Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

---

Exxon Biomedical Sciences, Inc. (1991b) Alkenes, C6: In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method. Conducted by Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

Exxon Biomedical Sciences, Inc. (1991c) Alkenes, C6: In vivo mammalian bone marrow micronucleus assay: inhalation dosing method. Conducted by Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

Exxon Biomedical Sciences, Inc. (1991d). Alkenes, C8-10, C9 Rich: Microbial Mutagenesis in *Salmonella*: Mammalian Microsome Plate Incorporation Assay. Conducted by Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

Exxon Biomedical Sciences, Inc. (1991e) Alkenes, C8-10, C9 Rich: In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method. Conducted by Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

Exxon Chemical Company (1993) Alkenes, C6-8, C7 Rich: In vivo mammalian bone marrow micronucleus assay: Oral gavage method. Conducted by Exxon Chemical Company (unpublished report).

ExxonMobil Biomedical Sciences, Inc. 2004. *Daphnia magna* Reproduction Test with 1-Decene. Conducted by ExxonMobil Biomedical Sciences, Inc., East Millstone, NJ, USA. Study # 180446 (unpublished report).

Gingell R, Bennick JE and Malley LA (1999). Subchronic inhalation study of 1-hexene in Fischer 344 Rats. *Drug and Chemical Toxicology* 22(3), 507-528.

Gingell R, Daniel EM, Machado M and Beven C. (2000). Reproduction/developmental toxicity screening test in rats with orally administered 1-hexene. *Drug and Chemical Toxicology* 23 (2), 327-338.

Goode, J.W. and Brecher, S. (1983a) GULFTENE 6: BALB/3T3 transformation test, Project 2072. Sponsored by Gulf Life Sciences Institute, Pittsburg, PA (unpublished report).

Goode, J.W. and Brecher, S. (1983b) GULFTENE 12-16: BALB/3T3 transformation test, Project 2070. Sponsored by Gulf Life Sciences Institute, Pittsburg, PA (unpublished report).

Gould ES (1959). *Mechanism and Structure in Organic Chemistry*. Holt, Reinhart and Winston.

Gulf Life Sciences Center (1983a). Two-week repeated dose toxicity study in rats using GULFTENE 12-16. Project No. 82-059. Conducted for Gulf Oil Chemicals Company (unpublished report).

Gulf Life Sciences Center (1983b). Micronucleus test in mouse bone marrow: GULFTENE 6 administered by inhalation using 2 daily 2-hour treatments. Project No. 82-119 (unpublished report).

Gulf Life Sciences Center (1983c) CHO/HGPRT Test: GULFTENE 12-16, Project 82-102. Conducted for Gulf Oil Chemicals Company, Pittsburg, Pennsylvania (unpublished study).

Gulf Life Sciences Center (1983d) Micronucleus Test in Mouse Bone Marrow with GULFTENE 12-16 Administered by Dermal Application for 2 Days. Gulf Oil Chemicals Company, Pittsburg, Pennsylvania, Sponsor (unpublished report).

Gulf Life Sciences (1984a) Hepatocyte Primary Culture/DNA Repair Test of GULFTENE 6, project #2071 (unpublished report).

Gulf Life Sciences (1984b) Hepatocyte Primary Culture/DNA Repair Test of GULFTENE 12-16, project #2069 (unpublished report).

Hard GC, Rodgers IS, Baetcke KP, Richards WL, McGaughy RE and Valcovic LR (1993). Hazard evaluation of chemicals that cause accumulation of alpha 2u-globulin, hyaline droplet nephropathy, and tubule neoplasia in the kidneys of male rats. *Environ. Health Perspect.* 99, 313-349.

Harris JC (1982a). Rate of Aqueous Photolysis. In: *Handbook of Chemical Property Estimation Methods*. Chapter 8 Edited by Lyman WJ, Reehl WF, and Rosenblatt DH. McGraw-Hill Book Company.

Harris, J.C. (1982b) Rate of Hydrolysis. In: *Handbook of Chemical Property Estimation Methods*. Chapter 7 Edited by Lyman WJ, Reehl WF, and Rosenblatt DH. McGraw-Hill Book Company.

Hazleton Laboratories America, Inc. (1982a). Neohexene: *Salmonella typhimurium* mammalian microsome plate incorporation assay. Conducted by Hazleton Laboratories America, Inc., for Phillips Petroleum Company (unpublished report).

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

---

Hoekstra WG and PH Phillips (1963). Effects of topically applied mineral oil fractions on the skin of Guinea pigs. *J. Invest. Derm.* 40(2):79-88.

Huntingdon Research Center (1990a). 1-Hexene: Bacterial Mutation Assay. Sponsored by Ethyl (unpublished report).

Huntingdon Research Center (1990b). 1-Hexene In Vitro Mammalian Cell Gene Mutation Assay (TK+/-). Sponsored by Ethyl (unpublished report).

Huntingdon Research Center (1990c). 1-Hexene: Metaphase chromosome analysis of human lymphocytes cultured in vitro. Sponsored by Ethyl (unpublished report).

Mackay D (1991). *Multimedia Environmental Models: The Fugacity Approach*. Lewis Publishers Inc., CRC Press, 67-183.

Mackay D, Di Guardo A, Paterson S, Kicsi G, and Cowan CE (1996a). Assessing the fate of new and existing chemicals: a five-stage process. *Environ. Toxicol. Chem.* 15(9), 1618-1626.

Mackay D, Di Guardo A, Paterson S, and Cowan CE (1996b). Evaluating the environmental fate of a variety of types of chemicals using the EQC model. *Environ. Toxicol. Chem.* 15(9), 1627-1637.

Maynert EW, Foreman RL and Watabe T (1970). Epoxides as obligatory intermediates in the metabolism of olefins to glycols. *J. Biol. Chem.* 245, 5234-5238.

McCarty LS and Mackay D (1993). Enhancing ecotoxicological modeling and assessment. *Environmental Science and Technology* 27, 1719-1728.

McCarty LS, Mackay D, Smith AD, Ozburn GW, and Dixon DG (1991). Interpreting aquatic toxicity QSARs: The significance of toxicant body residues at the pharmacologic endpoint. **In:** *WSAR in Environmental Toxicology - IV*. Edited by Hermens JLM and Opperhuizen J. Elsevier.

Neely WB (1985). Hydrolysis. **In:** *Environmental Exposure from Chemicals*. Volume I. Edited by Neely WB and Blau GE. CRC Press, 157-173.

NLM (2003a). TRI (Toxic Release Inventory). U.S. National Library of Medicine, Specialized Information Services, National Institutes of Health, Department of Health and Human Services. September 2003 (<http://toxnet.nlm.nih.gov>).

NLM (2003b). Household Products Database. U.S. National Library of Medicine, Specialized Information Services, National Institutes of Health, Department of Health and Human Services. September, 2003. (<http://toxnet.nlm.nih.gov>).

Oesch F (1973). Mammalian epoxide hydrases: inducible enzymes catalysing the inactivation of carcinogenic and cytotoxic metabolites derived from aromatic and olefinic compounds. *Xenobiotica* 3(5), 305-340.

Ortiz de Montellano PR and Mico BA (1980). Destruction of cytochrome P-450 by ethylene and other olefins. *Molec. Pharmacol.* 18, 128-135.

Pitter P and Chudoba J (1990). *Biodegradability of Organic Substances in The Aquatic Environment*, CRC Press.

Research Institute of Organic Synthesis a.s (1990). Pardubice, Czech Republic, Report No. T2129 (unpublished report).

Schulte-Hermann R (1974). Induction of liver growth by xenobiotic compounds and other stimuli. *Crit. Rev. Toxicol.* 3, 97-158.

Shell Development Company (1983a) In Vitro Chromosome Aberration Assay in Chinese Hamster Cells of NEODENE 6 Alpha Olefin, WTP-126 (unpublished report).

Shell Development Company, Westhollow Research Center (1983b) Assay of NEODENE-8 Alpha Olefin for Gene Mutation in *Salmonella typhimurium* (unpublished report).

Shell Development Company, Westhollow Research Center (1983c) In Vitro Chromosome Aberration Assay in Chinese Hamster Cells of NEODENE 8 Alpha Olefin (unpublished report).

Shell Development Company, Westhollow Research Center (1983d) Cell Transformation Assay of NEODENE-8 Alpha Olefin in the Absence and Presence of Microsomal Activation. Performed at Litton Bionetics, Inc., (unpublished report).

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

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- Shell Development Company (1984). *In vitro* destruction of hepatic cytochrome P-450 and heme by NEODENE 6 Alpha Olefin, WRC-814 (unpublished report).
- Shell Oil Company (1992a). Evaluation of primary irritation potential of Neodene 18 in humans. Single 24 hour application. Report 92-1388-70A (unpublished report).
- Shell Oil Company (1992b). Repeated insult patch test of Neodene 18 in humans. Report 92-1388-70B (unpublished report).
- Sipes IG and Gandolfi AJ (1991). Biotransformation of toxicants. In (1991). Cassarett and Doull's Toxicology. 4th ed. Edited by Amdur MO, Soull J, and Klassen CD. Pergammon Press, 88-126.
- SRI (2000). Chemical Economics Handbook. SRI International. Menlo Park, CA. September 2000.
- SRI (2001). Chemical Economics Handbook. SRI International. Menlo Park, CA. August 2001.
- Swann RL, Laskowshi DA, McCall PJ, Vander-Kuy K and Disburger HJ (1983). A rapid method for the estimation of the environmental parameters octanol/water partition coefficient, soil sorption constant, water to air ratio and water solubility. *Residue Reviews* **85**, 17-28.
- Thompson PW (1998a) C20-24 Alkenes, Branched and Linear: Salmonella typhimurium and Escherichia coli/Mammalian-Microsome Reverse Mutation Assay, SafePharm Laboratories Limited Project No. 703/086. Conducted for Chevron Research and Technology Company (unpublished report).
- Thompson PW (1998b) C24-30 Alkenes, Branched and Linear: Salmonella typhimurium and Escherichia coli/Mammalian-Microsome Reverse Mutation Assay, SafePharm Laboratories Limited Project No. 703/87. Conducted for Chevron Research and Technology Company (unpublished report).
- Thorsrud BA (2003a). A combined repeated dose toxicity study and reproduction/developmental screening study in Sprague Dawley rats with (C6) alkenes. Report No. 3604.2. Conducted by Springborn Laboratories, Spencerville, OH, for American Chemistry Council Higher Olefins Panel (unpublished study).
- Thorsrud BA (2003b). An oral (gavage) reproduction/ developmental toxicity screening study in Sprague Dawley rats with (C18) Octadecenes. Report No. 3604.1. Conducted by Springborn Laboratories, Spencerville, OH, for American Chemistry Council Higher Olefins Panel (unpublished study).
- Til HP et al. (1986). Sub-chronic (90-day) oral toxicity study with octene-1 in rats. Conducted by Civo Institutes TNO, Report No. V86.408/251091 for DSM, Beek, the Netherlands, Project No. B85-1091 (unpublished report).
- Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at <http://www.trentu.ca/cemc>)
- US EPA (1999a). Determining the Adequacy of Existing Data. OPPT, EPA.(found at [www.epa.gov/chemrtk/guidocs.htm](http://www.epa.gov/chemrtk/guidocs.htm))
- US EPA (1999b). The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA. (found at [www.epa.gov/chemrtk/guidocs.htm](http://www.epa.gov/chemrtk/guidocs.htm))
- Van Wezel AP and Opperhuizen A (1995). Narcosis due to environmental pollutants in aquatic organisms: residue-based toxicity, mechanisms, and membrane burdens. *Critical Reviews in Toxicology* **25**, 255-279.
- Verbruggen EMJ, Vaes WJJ, Parkerton TF and Hermens JLM (2000). Polyacrylate-coated SPME fibers as a tool to simulate body residues and target concentrations of complex organic mixtures for estimation of baseline toxicity. *Environmental Science and Technology* **34**, 324-331.
- Watabe T and Maynert EW (1968). *Pharmacologist* **10**,203 as cited in Watabe, T. and N. Yamada (1975). The biotransformation of 1-hexadecene to carcinogenic 1,2-epoxyhexadecane by hepatic microsomes. *Biochemical Pharmacology* **24**, 1051-1053.
- Watabe T and Yamada N (1975). The biotransformation of 1-hexadecene to carcinogenic 1,2-epoxyhexadecane by hepatic microsomes. *Biochemical Pharmacology* **24**, 1051-1053.
- Wilmer, J.W.G.M. (1986) Chromosome Analysis of Chinese Hamster Ovary Cells Treated in Vitro with 1-Octene. Conducted by Civo Institutes TNO, Report No. V 86.168/251124, for DSM, Geleen, the Netherlands, Project No. B 85-1124 (Unpublished report).

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

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Wright NP (1998) C20-24 Alkenes, Branched and Linear: Chromosome Aberration Test in Human Lymphocytes In Vitro, SafePharm Laboratories Limited Project No. 703/122. Conducted for Chevron Research and Technology Company (unpublished report).

Zahlsen K, Eide I, Nilsen AM and Nilsen OG (1993). Inhalation kinetics of C8-C10 1-alkenes and iso-alkanes in the rat after repeated exposures. *Pharmacology & Toxicology* 73, 163-168.

**NOTE: References for studies cited in the Category Summary are included in this report. However, the Dossiers provide a comprehensive listing of references.**

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Annex to Category Summary

**Table 1** Environmental fate and transport of the Higher Olefins Category members and selected C<sub>6</sub>-C<sub>54</sub> alpha and internal olefin components of category members.<sup>a</sup> [Note: Data for individual alpha or internal olefins that are not category members but are components of category members are shown as surrogates for category members that are olefin blends. Category members are shown in bold type]

Chemical	WWTP <sup>b</sup> % removal	Distribution fugacity level III <sup>c</sup> (Constant loading)	Distribution fugacity level I <sup>d</sup> (Equilibrium)	Henry's Law Constant (atm·m <sup>3</sup> /mole) <sup>e</sup>	Organic/carbon partition coefficient (K <sub>oc</sub> )	Atmospheric oxidation T1/2	Volatilization from water T1/2
<b>C6: Hexene</b>	>99%	Air = 2.9% Water= 90.6% Soil= 5.8% Sediment= <1%	Air = 100% Water = <1% Soil = < 1% Sediment = <1%	0.423 (B) 0.370 (G) 0.383 (U)	149	-OH = 2.2 hrs [cis] -OH = 1.9 [trans] O3 = 2.1 hrs [cis] O3 = 1.4 hrs [trans]	River = 0.9 hrs Lake = 3.6 days
<b>C6: Neohexene</b>	>99%	Air = 12.4% Water= 84.9% Soil= 1.8% Sediment= <1%	Air = 100% Water = <1% Soil = < 1% Sediment = <1%	0.359 (B) not estimated (G) 0.498 (U)	96.6	-OH = 4.8 hrs O3 = 6.5 days	River = 0.9 hrs Lake = 3.6 days
<b>C7: Heptene</b>	>99 %	Air = 7.7% Water= 79.5% Soil= 11% Sediment= 1.6%	Air = 100% Water = <1% Soil = < 1% Sediment = <1%	0.476 (B) 0.756 (G) 0.538 (U)	275	-OH = 4.1 hrs O3 = 22.9 hrs	River = 1.0 hrs Lake = 3.9 days
<b>C8: Octene</b>	>99 %	Air = 7.4% Water= 69.2% Soil= 17.4% Sediment= 5.9%	Air = 100% Water = <1% Soil = < 1% Sediment = <1%	0.632 (B) 1.07 (G) 0.667 (U)	507	-OH = 3.9 hrs O3 = 22.9 hrs	River = 1.1 hrs Lake = 4.2 days
<b>C9: Nonene</b>	>99 %	Air = <1% Water= 41.2% Soil= 52.6% Sediment= 5.2%	Air = 99% Water = <1% Soil < 1% Sediment = <1%	0.99 (B) 1.04 (G) 0.241 (U)	935	-OH = 2.0 hrs [cis] -OH = 1.8 hrs [trans] O3 = 2.1 hrs [cis] O3 = 1.4 hrs [trans]	River = 1.1 hrs Lake = 4.4 days

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical	WWTP <sup>b</sup> % removal	Distribution fugacity level III <sup>c</sup> (Constant loading)	Distribution fugacity level I <sup>d</sup> (Equilibrium)	Henry's Law Constant (atm·m <sup>3</sup> /mole) <sup>e</sup>	Organic/carbon partition coefficient (K <sub>oc</sub> )	Atmospheric oxidation T1/2	Volatilization from water T1/2
C10: Decene [component of category member]	>99	Air = 1.3% Water= 19.3% Soil= 36.3% Sediment= 43%	Air = 98.1% Water= <1% Soil=1.82% Sediment=<1%	1.11 (B) 2.13 (G) 1.17 (U)	1724	-OH = 3.6 hrs O3 = 22.9 hrs	River = 1.2 hrs Lake = 4.7 days
C10: 1-Decene [component of category member]	>99	Air = 1.1% Water= 17.9% Soil= 41.1% Sediment= 39.9%	Air = 96.1% Water= <1% Soil=3.9% Sediment=<1%	1.11 (B) 2.13 (G) 1.17 (U)  2.68[1-decene] (m)	1724	-OH = 3.6 hrs O3 = 22.9 hrs	River = 1.2 hrs Lake = 4.7 days
C11: Undecene [component of category member]	>99	Air =<1% Water= 26.7% Soil= 46.8% Sediment= 26.1%	Air = 95.9% Water= <1% Soil=4.04% Sediment=<1%	1.75 (B) 2.50 (G) 0.35 (U)	3179	-OH = 2.0 hrs [cis] -OH = 1.8 hrs [trans] O3 = 2.1 hrs [cis] O3 = 1.4 hrs [trans]	River = 1.3 hrs Lake = 4.9 days
C12: Dodecene	>99%	Air = <1% Water= 13.0% Soil= 33.9% Sediment= 52.5%	Air = 89.4% Water = <1% Soil = 10.3% Sediment = <1%	1.96 (B) 4.25 (G) 0.475 (U)	5864	-OH = 3.3 hrs O3 = 22.9 hrs	River = 1.3 hrs Lake = 5.1 days
C12: 1-Dodecene [component of category member]	>99%	Air = <1% Water= 12.9% Soil= 34.5% Sediment= 52.0%	Air = 84.8% Water = <1% Soil = 14.9% Sediment = <1%	1.96 (B) 4.25 (G) 0.285 (U)	5864	-OH = 3.3 hrs O3 = 22.9 hrs	River = 1.3 hrs Lake = 5.1 days
Tridecene [component of category member]	>99%	Air = <1% Water= 9.8% Soil= 26.8% Sediment= 63%	Air = 79.9% Water = <1% Soil = 19.6% Sediment = <1%	2.61 (B) 6.00 (G) 0.69 (U)	10,800	-OH = 3.2 hrs O3 = 22.9 hrs	River = 1.4 hrs Lake = 5.3 days

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical	WWTP <sup>b</sup> % removal	Distribution fugacity level III <sup>c</sup> (Constant loading)	Distribution fugacity level I <sup>d</sup> (Equilibrium)	Henry's Law Constant (atm-m <sup>3</sup> /mole) <sup>e</sup>	Organic/carbon partition coefficient (K <sub>oc</sub> )	Atmospheric oxidation T1/2	Volatilization from water T1/2
C13: 1-Tridecene	>99%	Air = <1% Water= 9.8% Soil= 27.1% Sediment= 62.7%	Air = 70.7% Water = <1% Soil = 28.6% Sediment =<1%	2.61 (B) 6.00 (G) 0.69 (U)	10,800	-OH = 3.2 hrs O3 = 22.9 hrs	River = 1.4 hrs Lake = 5.3 days
C14: Tetradecene [component of category member]	>99%	Air = <1% Water= 13.7% Soil= 23.1% Sediment= 63%	Air = 66.5% Water = <1% Soil = 32.7% Sediment =<1%	4.08 (B) 5.87 (G) 0.88 (U)	19,900	-OH = 1.8 hrs [cis] -OH = 1.6 hrs [trans] O3 = 2.1 hrs [cis] O3 = 1.4 hrs [trans]	River = 1.4 hrs Lake = 5.5 days
C14: 1-Tetradecene [component of category member]	99%	Air = <1% Water= 8.5% Soil= 24.0% Sediment= 67.2%	Air = 24.4% Water = <1% Soil = 73.9% Sediment = 1.6%	3.46 (B) 8.48 (G) 9.69 (U)	19,900	-OH = 3.1 hrs O3 = 22.9 hrs	River = 1.4 hrs Lake = 5.5 days
C15: Pentadecene [component of category member]	>99%	Air = <1% Water= 12.9% Soil= 21.6% Sediment= 65.4%	Air = 46.8% Water = <1% Soil = 52.0% Sediment = 1.2%	5.42 (B) 8.29 (G) 1.21 (U)	36,790	-OH = 1.8 hrs [cis] -OH = 1.6 hrs [trans] O3 = 2.1 hrs [cis] O3 = 1.4 hrs [trans]	River = 1.5 hrs Lake = 5.7 days
C16: Hexadecene [component of category member]	98%	Air = <1% Water= 12.7% Soil= 21.0% Sediment= 66.1%	Air = 30.6% Water = <1% Soil = 67.8% Sediment = 1.5%	7.2 (B) 11.7 (G) 1.8 (U)	67,900	-OH = 1.8 hrs [cis] -OH = 1.6 hrs [trans] O3 = 2.1 hrs [cis] O3 = 1.4 hrs [trans]	River = 1.5 hrs Lake = 5.9 days
C16: 1-Hexadecene	95%	Air = <1% Water= 7.9% Soil= 22.4% Sediment= 69.4%	Air = 9.6% Water = <1% Soil = 88.4% Sediment = 2%	6.1 (B) 16.9 (G) 0.541 (U)	67,900	-OH = 2.9 hrs O3 = 22.9 hrs	River = 1.5 hrs Lake = 5.9 days

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical	WWTP <sup>b</sup> % removal	Distribution fugacity level III <sup>c</sup> (Constant loading)	Distribution fugacity level I <sup>d</sup> (Equilibrium)	Henry's Law Constant (atm·m <sup>3</sup> /mole) <sup>e</sup>	Organic/carbon partition coefficient (K <sub>oc</sub> )	Atmospheric oxidation T1/2	Volatilization from water T1/2
C18: Octadecene [component of category member]	95%	Air = <1 Water= 7.9% Soil= 22.2% Sediment= 69.7%	Air = 12.5% Water = <1% Soil = 85.5% Sediment = 1.9%	10.7 (B) 33.8 (G) 6.9 (U)	230,800	-OH = 2.7 hrs O3 = 22.9 hrs	River = 1.6 hrs Lake = 6.3 days
C18: 1-Octadecene	95%	Air = <1 Water= 7.9% Soil= 22.3% Sediment= 69.6%	Air = <1% Water = <1% Soil = 97.5% Sediment = 2.2%	10.7 (B) 33.8 (G) 0.149 (U)	230,800	-OH = 2.7 hrs O3 = 22.9 hrs	River = 1.6 hrs Lake = 6.3 days
C20: 1-Eicosene	94%	Air = <1 Water= 7.8% Soil= 22.4% Sediment= 69.5%	Air = <1% Water = <1% Soil = 97.7% Sediment = 2.2%	18.9 (B) 67.4 (G) 11.9 (U)	785,200	-OH = 2.6 hrs O3 = 22.9 hrs	River = 1.7 hrs Lake = 6.6 days
C22: 1-Docosene	94%	Air = <1 Water= 7.9% Soil= 22.2% Sediment= 69.7%	Air = <1% Water = <1% Soil = 97.2% Sediment = 2.2%	33.4 (B) 134 (G) 27.9 (U)	2,671,000	-OH = 2.4 hrs O3 = 22.9 hrs	River = 1.8 hrs Lake = 7.0 days
C24: 1-Tetracosene	94%	Air = <1 Water= 7.9% Soil= 22.3% Sediment= 69.7%	Air = <1% Water = <1% Soil = 97.7% Sediment = 2.2%	58.8 (B) 268 (G) 41.0 (U)	9,086,000	-OH = 2.3 hrs O3 = 22.9 hrs	River = 1.9 hrs Lake = 7.3 days
C26: 1-Hexacosene [component of category member]	94%	Air = <1 Water= 3.5% Soil= 27.2% Sediment= 69.2%	nda <sup>f</sup>	104 (B) 535 (G) 85.0 (U)	30,910,000	-OH = 2.2 hrs O3 = 22.9 hrs	River = 1.9 hrs Lake = 7.6 days

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical	WWTP <sup>b</sup> % removal	Distribution fugacity level III <sup>c</sup> (Constant loading)	Distribution fugacity level I <sup>d</sup> (Equilibrium)	Henry's Law Constant (atm-m <sup>3</sup> /mole) <sup>e</sup>	Organic/carbon partition coefficient (Koc)	Atmospheric oxidation T1/2	Volatilization from water T1/2
C28: 1-Octacosene [component of category member]	94%	Air = <1 Water= 3.5% Soil= 27.5% Sediment= 68.9%	nda <sup>f</sup>	183 (B) 1070 (G) 172 (U)	105,100,000	-OH = 2.1 hrs O3 = 22.9 hrs	River = 2.0 hrs Lake = 7.8 days
C30: 1-Triacontene [component of category member]	94%	Air = <1 Water= 3.4% Soil= 28% Sediment= 68.5%	nda <sup>f</sup>	322 (B) 2130 (G) 341 (U)	357,700,000	-OH = 2.0 hrs O3 = 22.9 hrs	River = 2.1 hrs Lake = 8.1 days
C54 alpha olefin [component of category member]	94%	Air = <1 Water= 2.4% Soil= 29.2% Sediment= 68.4%	nda <sup>f</sup>	2.89[E5] (B) 8.48[E6] (G) 1.574[E7] (U)	10,000,000,000	-OH = 1.3 hrs O3 = 22.9 hrs	River = 2.8 hrs Lake = 10.89 days

<sup>a</sup> All values calculated using EPIWIN, v.3.11 (EPIWIN, 2000b), except as noted. Calculations used CAS number input and associated alpha olefin structures except for those for hexene, nonene, undecene, tetradecene and hexadecene which used structures for internal olefins.

<sup>b</sup> WWTP = Waste Water Treatment Plant

<sup>c</sup> Level III Model, Trent University, used for all substances except for those with carbon chain lengths  $\geq$  C26, for which the EPIWIN Level III Model (EPIWIN, 2000b) was used. The Trent University model did not appear to be suitable for the olefins with  $\geq$ 26 carbon atoms. Partitioning reflects constant loading to air, water and soil compartments (1000 kg/hr to each). Values for environmental half-lives were taken from EPIWIN results.

<sup>d</sup> Level I Model, Trent University. Partition reflects equilibrium among all compartments.

<sup>e</sup> Henry's Law Constant estimated using EPIWIN. Estimates are provided using Bond (B) method, Group (G) method, and User- or EPIWIN supplied vapor pressure and water solubility (U).

<sup>f</sup> nda: No data available - values were not calculated because the Trent University model did not appear to be suitable for this substance.

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Table 2: Health effects (SIDS endpoints) for Higher Olefins Category members and analogues/surrogates<sup>a</sup>

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
C6  All studies appear in the hexene dossier	<p><u>1-hexene and neohexene:</u> Oral: Rat LD50&gt;5.6 g/kg [1-hexene]; &gt;5 g/kg [neohexene]</p> <p>Inhalation: Rat LC50 (4hr) = 110 mg/L (32,000 ppm, nom) [1-hexene]; &gt;176 mg/L (51,000 ppm) [neohexene]</p> <p>Dermal: Rabbit LD50 &gt;2 g/kg [1-hexene]</p>	<p><u>alkenes, C6 (internal branched stream):</u> Rat oral OECD 422; dosed at 0, 100, 500, 1000 mg/kg/day; NOAEL = 1000 mg/kg/day; NOEL = 100 mg/kg/day (females, kidney effects); not determined for males due to kidney and adrenal effects.</p> <p><u>1-hexene:</u> Rat, 90-day inhalation OECD 413; exposed to 0, 1.03, 3.44, 10.33 mg/L (0, 300, 1000, 3000 ppm); NOEL= 3.44 mg/L (1000 ppm) (reduced bodyweight [females] and questionable organ weight changes);  Rat, 28-day gavage OECD 407; dosed at 0, 10, 101, 1010, 3365 mg/kg/day; NOEL=101 mg/kg/day (kidney effects - males); 1010 mg/kg/day (gastric effects and spleen weight - females)</p> <p>Rat oral OECD 421; dosed</p>	<p><u>alkenes, C6 (internal branched stream):</u> <i>S. typhimurium</i>, OECD 471, negative with and w/out activation</p> <p><u>1-hexene:</u> <i>S. typhimurium</i>, OECD 471; Mouse Lymphoma, OECD 476, Mammalian Cell gene mutation ; CHO and Human lymphocytes-Metaphase Chromosome Analysis, OECD 473. All negative with and w/out activation</p> <p>UDS-rat hepatocyte; OECD 482 w/out repeat assay; Negative</p> <p>BALB/3T3 transformation: Negative</p> <p><u>neohexene:</u> <i>S. typhimurium</i>, OECD 471 w/out repeat assay and CHO SCE, OECD 479, negative with and w/out activation</p>	<p><u>alkenes, C6 (internal branched stream) and 1-hexene:</u> Mouse Bone Marrow micronucleus, OECD 474 (inhl); negative at 0, 3.44, 34.42, 86.05 (0, 1000, 10000 and 25000 ppm) [1-hexene] and 3.64 mg/L (1057 ppm) [Alkenes, C6]</p> <p><u>alkenes, C6 (internal branched stream):</u> Mouse Bone Marrow micronucleus, OECD 474 (oral); weakly positive at 5 g/kg</p>	<p><u>alkenes, C6 (internal branched stream):</u> Rat oral OECD 422; dosed at 0, 100, 500, 1000 mg/kg/day; NOAEL = 1000 mg/kg/day (reproductive and developmental toxicity)</p> <p><u>1-hexene:</u> Rat; OECD 421; oral dosed at 0, 100, 500, and 1000 mg/kg/day; NOEL&gt;1000 mg/kg/day (reproductive/developmental toxicity)</p> <p><u>1-hexene:</u> Rat; OECD 413; 90-day inhalation exposed to 0, 1.03, 3.44, 10.33 mg/L (0, 300, 1000, 3000 ppm); NOEL = 3.44 mg/L (1000 ppm) (questionable increases in testes weights)</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
		at 0, 100, 500, 1000 mg/kg/day; NOEL <100 mg/kg/day for males (kidney effects); 1000 mg/kg/day for females			
C7  All studies appear in the heptene dossier	<u>alkenes, C6-8, C7 rich (internal stream):</u> Inhalation: Rat, mouse and guinea pig LC50 (6hr) >42.3 mg/L (10,533 ppm)  Dermal: Rabbit LD50 >3160 mg/kg (24 hr)			<u>alkenes, C6-8, C7 rich (internal stream):</u> Mouse Bone Marrow micronucleus, EPA OTS 798.5395; (oral); negative at 1.25, 2.5 and 5 g/kg	
C8  All studies appear in the octene dossier	<u>1-octene and alkenes, C7-9, C8 rich internal stream:</u> Oral: Rat LD50>5 g/kg [1-octene]; >5g/kg [alkenes, C7-9, C8 rich internal stream]  Inhalation: Rat LC50 (4 hr) = 36.9 mg/L (8,050 ppm, nom) [1-octene]; rat and mouse LC50 (6 hr) > 31.7 mg/L (6900 ppm) and guinea pig LC50 (6 hr) < 31.7 mg/L (6900 ppm) [alkenes, C7-9, C8 rich internal stream]  Dermal: Rabbit LD50 > 1.43 g/kg (24 hr) [1-octene]; >3.16 g/kg (24 hr) [alkenes, C7-9, C8 rich	<u>1-octene:</u> Rat, 90 day oral (gavage) dosing at 0, 5, 50 or 500 mg/kg/day; NOEL = 50 mg/kg/day (between 50 and 500, probably only slightly less than 500) (increased kidney weights and decreased plasma chloride in both sexes); LOEL = 500 mg/kg/day	<u>1-octene:</u> <i>S. typhimurium</i> Ames Test and BALB/c-3T3 transformation: Negative with and w/out activation  Two CHO chromosome aberrations tests; one was negative with and w/out activation and the other had questionable results with activation; (aberration rate increased approx 2-fold over background, but no dose response) and was negative w/out activation.		

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
	internal stream]				
C9 All studies appear in the nonene dossier	<u>alkenes, C8-10, C9 rich (internal stream):</u> Oral: Rat LD50>2332 mg/kg  Inhalation: rat, mice, guinea pig LC50 (6 hr) > 11.1 mg/L (2150 ppm)  Dermal: Rabbit LD50 >2332 mg/kg (24 hr)		<u>alkenes, C8-10, C9 rich (internal stream):</u> <i>S. typhimurium</i> EPA OTS 798.5265: Negative with and w/out activation	<u>alkenes, C8-10, C9 rich (internal stream):</u> Mouse Bone Marrow micronucleus, EPA OTS 798.5395 (oral); negative at doses of 1.25, 2.5 and 5 g/kg	
C10 All studies appear in the decene dossier	<u>1-decene:</u> Oral: Rat LD50>10g/kg  Inhalation: Rat LC50 >saturation conc. for 1 and 4 hr exposures at saturation of 9.3 and 8.7 mg/L (1621 and 1516 ppm)  Dermal: Rabbit LD50 >10 g/kg (24 hr)		<u>1-decene:</u> <i>S. typhimurium</i> ; OECD 471; Negative with and w/out activation		
C10-13 All studies appear in the alkenes, C11-C13 dossier	<u>C10-13 internal olefins:</u> Oral: Rat LD50>7.74g/kg  Inhalation: Rat LC50 >2.1 mg/L (~305 ppm) (saturation conc.) for 4 hr exposure  Dermal: Rat LD50 >3080		<u>C10-13 internal olefins:</u> <i>S. typhimurium</i> and <i>E. Coli</i> Ames Test; Negative with and w/out activation  Chromosome aberration test with rat liver RL1 cells: Negative		

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
	<p>mg/kg (24 hr)</p> <p><u>C13 internal olefin:</u> Oral: LD50&gt;5 g/kg</p> <p>Dermal: Rat LD50 &gt; 2 g/kg</p>				
<p>C12</p> <p>All studies appear in the C11-C13 dossier</p>	<p><u>1-dodecene; C12, 14, 16 linear AO blend; and alkenes, C11-13, C12 rich:</u> Oral: Rat LD50 &gt;10g/kg [1-dodecene]; &gt;7.74 g/kg [alkenes, C11-13, C12 rich internal stream]</p> <p>Inhalation: Rat LC50 (1hr) &gt;9.9 mg/L (1438 ppm) [C12, 14, 16 linear AO blend]; rat, mouse and guinea pig LC50 (6 hr) &gt; 4.4 mg/L (639 ppm) [alkenes, C11-13, C12 rich internal stream]</p> <p>Dermal: Rabbit LD50 &gt; 10 g/kg (24 hr)[C12-16 AO blend] and rat &gt;10 g/kg (24 hr)[1-dodecene]; rabbit LD50 &gt;2446 mg/kg (24 hr) [alkenes, C11-13, C12 rich internal stream]</p>	<p><u>C12, 14, 16 linear AO blend:</u> Dermal: Rat; 9 applications (6 hr) over 2 wk period of 1 or 2 g/kg/day; severe irritation and decrease in body and organ weights seen with 2 g/kg/day; slight irritation seen with 1 g/kg; NOAEL (systemic) = 1 g/kg/day</p>	<p><u>1-dodecene; C12, 14, 16 linear AO Blend; and C11-12 AO blend:</u> <i>S. typhimurium</i> and <i>E.coli</i> Ames Test [1-dodecene]; CHO/HGPRT [C12, C14, C16 linear AO blend]; <i>S. cerevisiae</i> Mitotic Gene conversion Assay [C11-12 AO blend]: All negative with and w/out activation</p> <p>Chromosome aberration test with rat liver RL1 cells [1-dodecene]; BALB/3T3 Mouse embryo transformation and UDS [C12, 14, 16 linear AO blend]: All negative</p>	<p><u>C12, 14, 16 linear AO blend:</u> Mouse Micronucleus Bone Marrow Test (dermal); No remarkable clinical findings-negative at doses of 1000, 2500 and 5000 mg/kg for 2 days</p>	
C14	<p><u>C12-14 AO blend, C14-16 AO blend, and C12, 14, 16</u></p>	<p><u>1-tetradecene:</u> Combined OECD 422; rat; gavage dosed at 0, 100, 500</p>	<p><u>C12, 14, 16 linear AO blend:</u> UDS (rat hepatocyte),</p>	<p><u>C12, 14, 16 linear AO blend:</u> Mouse Micronucleus</p>	<p><u>1-tetradecene:</u> Rat; Modified OECD 422; gavage at 0, 100, 500 or</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
All studies appear in the C14-C16 dossier	<p><u>linear AO blend:</u> Oral: Rat LD50 &gt;10g/kg [C12-14, C14-16 AO blends]</p> <p>Inhalation: Rat LC50 (1hr) &gt;9.9 mg/L (1438 ppm) [C12, 14, 16 linear AO blend]</p> <p>Dermal: Rabbit LD50 &gt;10 g/kg (24 hr) [C12-14 and C14-16 AO blends]</p>	<p>or 1000 mg/kg/day for up to 51 days. NOEL = 100 mg/kg/day for females(liver effects); no NOEL for males due to kidney effects</p> <p><u>C12, 14, 16 linear AO blend:</u> Dermal: Rat; 9 applications (6 hr) over 2 wk period of 1 or 2 g/kg/day; severe irritation and decrease in body and organ weights seen with 2 g/kg/day; slight irritation seen with 1 g/kg; NOAEL (systemic) = 1 g/kg/day</p>	<p>CHO HGPRT and BALB/3T3 transformation: Negative</p>	<p>Assay (dermal); Negative at doses of 1000, 2500 and 5000 mg/kg for 2 days.</p>	<p>1000 mg/kg/day for up to 51 days; NOAEL (reproductive and developmental toxicity) = 1000 mg/kg/day</p>
C16 All studies appear in the C14-C16 dossier	<p><u>1-hexadecene and C16 internal linear and branched:</u> Oral: Rat LD50 &gt;10g/kg [1-hexadecene] and &gt;5050 mg/kg [C16 internal linear and branched]</p> <p>Inhalation: Rat LC50 = 6.4 mg/L (693 ppm) (4hr) and &gt;8.5 mg/L (926 ppm) (1 hr) [1-hexadecene]</p> <p>Dermal: Rabbit LD50 &gt;2020 mg/kg (24 hr) [C16 internal linear and branched]</p>	<p><u>C16/18 internal linear and branched:</u> Oral: OECD 407; rat; dosed at 0, 25, 150 or 1000 mg/kg/day for up to 4 wks. NOAEL = 1000 mg/kg/day</p> <p><u>C12, 14, 16 linear AO blend:</u> Dermal: Rat; 9 applications (6 hr) over 2 wk period of 1 or 2 g/kg/day; severe irritation and decrease in body and organ weights seen with 2 g/kg/day; slight irritation seen with 1 g/kg; NOAEL (systemic) = 1</p>	<p><u>1-hexadecene:</u> OECD 471, <i>S. typhimurium</i>: Negative with and w/out activation</p> <p><u>C12, 14, 16 linear AO blend:</u> UDS (rat hepatocyte), CHO HGPRT and BALB/3T3 transformation: Negative</p>	<p><u>1-hexadecene:</u> OECD 474, Mouse Micronucleus Assay (oral); Negative at 7.85 g/kg (only dose administered).</p> <p><u>C12, 14, 16 linear AO blend:</u> Mouse Micronucleus Assay (dermal); Negative at doses of 1000, 2500 and 5000 mg/kg for 2 days.</p>	<p><u>C16/18 internal linear and branched:</u> Oral: OECD 407; rat; dosed at 0, 25, 150 or 1000 mg/kg/day for up to 4 wks; NOAEL for reproductive effects from limited data (effect on reproductive organs) = 1000 mg/kg/day</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
	branched]	g/kg/day			
C18  All studies appear in the C18-C54 dossier	<p><u>various AO blends and C18 internal linear and branched:</u> Oral: Rat LD50 &gt;10g/kg [C14-18 AO blend, C18-26 AO blend, C18-24 AO blend] and &gt;5050 mg/kg [C18 internal linear and branched]</p> <p>Dermal: Rabbit LD50 &gt;10 g/kg (24 hr) [C18-24 AO blend, C18-26 AO blend] and &gt;2020 mg/kg (24 hr) [C18 internal linear and branched]</p>	<p><u>C16/18 internal linear and branched:</u> Oral: OECD 407; rat; dosed at 0, 25, 150 or 1000 mg/kg/day for up to 4 wks. NOAEL = 1000 mg/kg/day</p> <p><u>C18 internal linear and branched:</u> Oral: OECD 421; rat; dosed at 0, 100, 500 and 1000 mg/kg/day; NOAEL (general toxicity – limited endpoints) = 1000 mg/kg /day</p>	<p><u>1-octadecene:</u> <i>S. cerevisiae</i> Mitotic gene conversion and <i>S. typhimurium</i> and <i>E. coli</i> Ames Test with and w/out activation; Chromosome aberration test with Rat Liver RL1 cells: Negative</p>		<p><u>C18 internal linear and branched:</u> Oral: OECD 421; rat; dosed at 0, 100, 500 and 1000 mg/kg/day; NOAEL (reproductive/developmental toxicity) = 1000 mg/kg /day</p> <p><u>C16/18 internal linear and branched:</u> Oral: OECD 407; rat; dosed at 0, 25, 150 or 1000 mg/kg/day for up to 4 wks; NOAEL for reproductive effects from limited data (effect on reproductive organs) = 1000 mg/kg/day</p>
C20-24  All studies appear in the C18-C54 dossier	<p><u>C20-24 linear AO, C22-28 linear AO, C20-24 internal linear and branched:</u> Oral: Rat LD50 &gt;5 g/kg [C20-24 linear AO, C22-28 linear AO, C20-24 internal linear and branched] and &gt;15 g/kg [C20-24 linear AO]</p> <p>Dermal: rat LD50 &gt;5 ml/kg (24 hr) [C20-24 linear AO] and &gt;2 g/kg [C20-24 internal linear and</p>	<p><u>C20-24 internal linear and branched:</u> OECD 408; rat gavage dosed at 0, 100, 500 or 1000 mg/kg/day for 90 days with 4-wk recovery group. NOAEL = 1000 mg/kg/day; NOEL = 100 mg/k/day for males (glucose); NOEL = 500 mg/kg/day for females (liver weight and adrenal hypertrophy)</p>	<p><u>C20-24 internal linear and branched:</u> <i>S. typhimurium</i> and <i>E. coli</i> OECD 471; and OECD 473 Chromosome aberrations test with human lymphocytes: Negative with and w/out activation</p>	<p><u>C20-24 internal linear and branched:</u> OECD 474 Mouse Micronucleus Assay (i.p.): Negative at doses of 500, 1000 and 2000 mg/kg/day</p>	<p><u>C20-24 internal linear and branched:</u> Oral: OECD 408; rat; dosed at 0, 100, 500 or 1000 mg/kg/day for 90 days with a 4-wk recovery group; NOEL for reproductive effects from limited data (effect on reproductive organs) = 1000 mg/kg/day</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
	branched]				
<b>C24-30</b> All studies appear in the C18-C54 dossier	<u>C24-30 internal linear and branched:</u> Oral: Rat LD50 >5g/kg		<u>C24-30 internal linear and branched:</u> <i>S. typhimurium</i> OECD 471: negative with and w/out activation		
<b>C24-54 (C30+)</b> All studies appear in the C18-C54 dossier	<u>C24-54 AO linear and branched:</u> Oral: Rat LD50 >2g/kg and >15 g/kg  Dermal: rat LD50 >5 ml/kg (24 hr)				

<sup>a</sup> Study details and references are found in the robust summaries in the dossiers.

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

**Table 2a:** Irritation and sensitization data for Higher Olefins Category members and analogues/surrogates<sup>a</sup>

Carbon Number	Endpoint		
	Skin Irritation	Eye Irritation	Sensitization
<p><b>C6</b></p> <p>All studies appear in the C6 dossier</p>	<p><u>1-hexene:</u> OECD 404 [except that exposure was 24 hrs, occlusive dressing was used and skin was evaluated only at 24 and 72 hrs]; rabbit; Draize score = 0.975/8 OECD 404; rabbit; Draize = 0; not an irritant</p> <p><u>C6-8 internal olefins:</u> OECD 404; rabbit; semi-occlusive; very slight to slight erythema and edema (max. score = 2 at 48 hrs)</p>	<p><u>1-hexene:</u> OECD 405 [3 male and female unwashed, 3 male washed]; rabbit; Max individual animal Draize (1 hr) = 8/110 Max. Avg Draize (1 hr) = 5.0/110 (unwashed) Max. Avg Draize (1 hr) = 5.3/110 (washed)</p> <p><u>C6-8 internal olefins:</u> OECD 405 [3 rabbits]; scores for redness at 24 hr = 2, 1, 1; at 48 hr = 1, 0, 0; at 72 hr = 0; all other scores were zero</p>	<p><u>1-hexene:</u> OECD 406 – Buehler; guinea pig; negative</p> <p><u>C6-8 internal olefins:</u> OECD 406 – Magnusson and Kligman; guinea pig; negative</p>
<p><b>C7</b></p> <p>All studies appear in the C7 dossier</p>	<p><u>alkenes, C6-8, C7 rich:</u> Rabbit; 24 hr exposure, abraded skin, occlusive dressing; at 200 mg/kg, max. scores were 2.0 for erythema and 1.5 for edema (cleared by day 14); at 3160 mg/kg, max. scores were 3.0 for erythema and 2.3 for edema (persisted to day 14); irritant under these extreme testing conditions</p>	<p><u>alkenes, C6-8, C7 rich:</u> Rabbit; max. total Draize score = 15</p>	<p>No data</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Endpoint		
	Skin Irritation	Eye Irritation	Sensitization
<p><b>C8</b></p> <p>All studies appear in the C8 dossier</p>	<p><u>1-octene:</u> OECD 404; rabbit; PII = 4.2/8.0 (4-hr exposure); mean 24-72 hr score = 2.28 for erythema; max. score for edema = 1.83</p> <p>OECD 404; rabbit; semi-occluded; PII = 3.42/8.0; mean 24-72 hr scores = 1.9 for erythema and 1.1 for edema (4-hr exposure)</p> <p><u>alkenes, C7-9, C8 rich:</u> Rabbit; 24 hr exposure, abraded skin; at 200 and 3160 mg/kg; severe irritation observed</p>	<p><u>1-octene:</u> US FHSA method; rabbit; mean Draize score (unwashed) = 3.0/110 at 1 hr; 0.3 at 24 hr; 0.0 thereafter; (washed) = 4.7/110 at 1 hr, 0.0 thereafter</p> <p><u>alkenes, C7-9, C8 rich:</u> Rabbit; max. total Draize score = 4; conjunctival irritation cleared by 24 hr</p> <p><u>C6-8 internal olefin:</u> OECD 405; rabbit; very slight to slight conjunctival irritation cleared by 72 hr</p>	<p><u>1-octene:</u> Buehler; guinea pig; negative</p> <p><u>C6-8 internal olefin:</u> Magnusson and Kligman; guinea pig; negative</p>
<p><b>C9</b></p> <p>All studies appear in the C9 dossier</p>	<p><u>alkenes, C8-10, C9 rich:</u> Rabbit; 24 hr exposure, occlusive dressing; at 73.8, 233, 738 and 2332 mg/kg; mild erythema observed</p>	<p><u>alkenes, C8-10, C9 rich:</u> Rabbit; max. total Draize score = 6; mild conjunctival irritation cleared by 24 hr</p>	<p>No data</p>
<p><b>C10</b></p> <p>All studies appear in the C10 dossier</p>	<p><u>1-decene:</u> OECD 404; rabbit; semi-occluded; PII = 3.67/8.0; mean 24-72-hr scores = 2.0 for erythema and 1.7 for edema (4-hr exposure)</p> <p>US TSCA 40 CFR 798.4470; rabbit; occluded; irritation persisted at day 7 in 4/6 animals; PII = 5.3</p>	<p><u>1-decene:</u> OECD 405; rabbit; mean Draize score = 0.7/110 at 24 hr; 0.3 at 48 hr; 0 at 72 hr; max. individual score = 2/110 at 24 hr</p> <p>Rabbit; Draize score = 0.0; mean 24-72-hr scores for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis were 0, 0, 0.2, and 0, respectively</p>	<p>No data</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Endpoint		
	Skin Irritation	Eye Irritation	Sensitization
<p><b>C10-13</b> All studies appear in the C11-C13 dossier</p>	<p><u>C13 internal olefin:</u> US TSCA C40 CFR 798.4470; rabbit; occluded; PII = 3.5/8.0</p>	<p><u>C10-13 internal olefins:</u> Rabbit; mean Draize score = 0.9/110 at 24 hr; 0.1 at 48 hr; 0 at 72 hr</p>	<p><u>C10-13 internal olefins:</u> Magnusson and Kligman maximization; guinea pig; negative</p>
<p><b>C12</b> All studies appear in the C11-C13 dossier</p>	<p><u>1-dodecene:</u> OECD 404; rabbit; semi-occluded; PII = 4.67/8.0; mean 24-72-hr scores = 2.2 for erythema and 2.4 for edema (4-hr exposure); moderate to severe erythema and slight to severe edema; reversible on day 14</p> <p><u>alkenes, C11-13, C12 rich:</u> Rabbit; 24 hr exposure, occlusive dressing; at 77.4, 245, 774 and 2446 mg/kg; slight erythema at all doses cleared by 72 hr; slight edema at high dose which cleared by 48 hr; all signs cleared by day 12</p>	<p><u>1-dodecene:</u> Rabbit; Draize score = 2.5/110</p> <p><u>alkenes, C11-13, C12 rich:</u> Rabbit; max. total Draize score =10; very slight irritation in washed and unwashed eyes; cleared by 24 hr</p>	<p><u>C12-16 alpha olefins:</u> Modified Landsteiner method; guinea pig; negative</p>
<p><b>C14</b> All studies appear in the C14-C16 dossier</p>	<p><u>1-tetradecene:</u> OECD 404; rabbit; semi-occluded; PII = 2.79/8.0; mean 24-72-hr scores = 1.3 for erythema and 1.1 for edema (4-hr exposure)</p>	<p><u>C12-16 alpha olefins:</u> Rabbit; mean Draize score = 1.0/110 at 24 hr; 0.7 at 48 hr; 1.3 at 72 hr</p>	<p><u>C12-16 alpha olefins:</u> Modified Landsteiner method; guinea pig; negative</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Endpoint		
	Skin Irritation	Eye Irritation	Sensitization
<p><b>C16</b></p> <p>All studies appear in the C14-C16 dossier</p>	<p><u>1-hexadecene:</u> OECD 404; rabbit; semi-occluded; PII = 2.46/8.0; mean 24-72-hr scores = 1.3 for erythema and 0.9 for edema (4-hr exposure)</p> <p><u>C16-18 internal linear and branched:</u> OECD 404 except only 3 animals; rabbit; semi-occluded; PII = 2.2/8.0; mean 24-72-hr scores [for each animal] = 1.3, 2.0, 1.3 for erythema and 0.0, 0.3, 0.3 for edema (4-hr exposure)</p> <p><u>1-hexadecene:</u> Dermal: guinea pig; 4 exposures in 8 days; evaluated for 20 days after first exposure; treated site not covered or cleaned between applications; max. score of 8/8; severely irritating</p>	<p><u>1-hexadecene:</u> OECD 405; rabbit; mean Draize score = 1.3/110 at 24 hr; 0.3 at 48 hr; 0 at 72 hr; mean 24-72-hr scores for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis were 0, 0, 0.3, and 0, respectively</p> <p><u>C16-18 internal linear and branched:</u> OECD 405 except only 3 animals; rabbit; mean Draize score = 2.0/110 at 24 hr; mean 24-72-hr scores for each animal were 0 for corneal opacity and iritis, 0.0, 0.33, 0.33 for conjunctival redness, and 0.0, 0.33, 0.0 for conjunctival chemosis</p>	<p><u>1-hexadecene:</u> Buehler; guinea pig; negative</p> <p><u>C16-18 internal linear and branched:</u> Buehler; guinea pig; negative</p> <p><u>C12-16 alpha olefins:</u> Modified Landsteiner method; guinea pig; negative</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Endpoint		
	Skin Irritation	Eye Irritation	Sensitization
<p><b>C18</b></p> <p>All studies appear in the C18-C54 dossier</p>	<p><u>1-octadecene:</u> OECD 404; rabbit; semi-occluded; PII = 2.29/8.0; mean 24-72-hr scores = 1.5 for erythema and 0.9 for edema (4-hr exposure)</p> <p>US EPA TSCA 40 CFR; rabbit; occluded; PII = 3.2/8.0; mean 24-72-hr scores = 2.17 for erythema and 0.94 for edema (4-hr exposure)</p> <p>Human Patch Test; 24-hr exposure; semi-occluded patch on upper arm; applications of undiluted, 25%, 10%, 1% in mineral oil; no irritation with dilutions; strong clinical reactions with undiluted material</p> <p><u>C16-18 internal linear and branched:</u> OECD 404 except only 3 animals; rabbit; semi-occluded; PII = 2.2/8.0; mean 24-72-hr scores [for each animal] = 1.3, 2.0, 1.3 for erythema and 0.0, 0.3, 0.3 for edema (4-hr exposure)</p>	<p><u>C18-24 alpha olefin:</u> USA 16 CFR 1500.42 method; rabbit; mean Draize score = 4.67/110 at 24 hr; 2.0 at 48 hr; 0 at 72 hr; mean 24-72-hr scores for corneal opacity, iritis, conjunctival redness, and conjunctival chemosis were 0, 0, 0.50, and 0.61, respectively</p> <p><u>C16-18 internal linear and branched:</u> OECD 405 except only 3 animals; rabbit; mean Draize score = 2.0/110 at 24 hr; mean 24-72-hr scores for each animal were 0 for corneal opacity and iritis, 0.0, 0.33, 0.33 for conjunctival redness, and 0.0, 0.33, 0.0 for conjunctival chemosis</p>	<p><u>1-octadecene:</u> Buehler; guinea pig; negative</p> <p>Human Patch Test; semi-occluded patch on upper arm; applications of 25% in mineral oil; 24-hr exposures; 9 induction exposures during 3 weeks; challenged after 10-17 days rest; negative</p> <p><u>C16-18 internal linear and branched:</u> Buehler; guinea pig; negative</p>

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Carbon Number	Endpoint		
	Skin Irritation	Eye Irritation	Sensitization
<p><b>C20-24</b></p> <p>All studies appear in the C18-C54 dossier</p>	<p><u>C20-24 alpha olefin:</u> USA TSCA (40CFR); rabbit; occluded; PII = 2.7; mean 24-72-hour scores = 1.94 for erythema and 0.72 for oedema; mean scores on Day 7 = erythema 0.33, oedema 0.0 (4-hr exposure)</p> <p><u>C20-24 internal linear and branched:</u> OECD 404; rabbit; semi-occluded; all scores were zero (4-hr exposure)</p>	<p><u>C20-24 internal linear and branched:</u> OECD 405; rabbit; conjunctival redness noted in 3/6 treated eyes at the 1 hr observation; all treated eyes appeared normal at the 24 hr observation</p>	<p><u>C20-24 alpha olefin:</u> Buehler; guinea pig; negative</p> <p><u>C20-24 internal linear and branched:</u> Magnusson and Kligman Maximisation; guinea pig; negative</p>

<sup>a</sup>Study details and references are found in the robust summaries in the dossiers.

HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Table 3 Data summary matrix for the Higher Olefins Category members

Chemical	CAS #	Human Health Effects						Ecotoxicity			Environmental Fate				
		Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Developmental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydrolysis	Fugacity	Biodeg.
Hexene (ICCA)	25264-93-1 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C6	68526-52-3 Br. and Lin.	RA	√	√	√	√	√	√	√	√	SAR	TD	TD	CM	√
Neohexene	558-37-2 Branched	√	√	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Heptene (ICCA)	25339-56-4 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C6-8, C7 rich	68526-53-4	√	RA	√	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Octene (ICCA)	25377-83-7 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C7-9, C8 rich	68526-54-5 Linear	√	RA	RA	RA	RA	RA	√	RA	RA	SAR	TD	TD	CM	√
Nonene (ICCA)	27215-95-8 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C8-10, C9 rich	68526-55-6 Linear	√	√	√	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C9-11, C10 rich	68526-56-7 Linear	RA	RA	RA	RA	RA	RA	√	RA	RA	SAR	TD	TD	CM	√
Alkenes, C10-12, C11 rich	68526-57-8 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
C10,12 Olefin rich hydrocarbons	68514-32-9 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Dodecene (ICCA – not sponsored in US HPV)	25378-22-7 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C11-13, C12 rich	68526-57-8 Linear	√	RA	RA	RA	RA	RA	√	RA	RA	SAR	TD	TD	CM	√
Heavy polymerization naphtha (petroleum)	68783-10-8 Branched	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C10-16 alpha (even carbon numbers)	68855-58-3 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C10-16	68991-52-6	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA

## HPV CHEMICAL CATEGORY SUMMARY: HIGHER OLEFINS CATEGORY

Chemical	CAS #	Human Health Effects						Ecotoxicity			Environmental Fate				
		Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Developmental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydrolysis	Fugacity	Biodeg.
	Linear														
C12,14 Olefin rich hydrocarbons	68514-33-0 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Tridecene	2437-56-1 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C14-18 alpha (even carbon numbers)	68855-59-4 Linear	√	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C14-20 alpha (even carbon numbers)	68855-60-7 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C15-18	93762-80-2 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Hexadecene (ICCA)	629-73-2 Linear	√	√	√	RA	RA	RA	√	RA	√	SAR	TD	TD	CM	√
1-Octadecene (ICCA)	112-88-9 Linear	RA	√	√	RA	RA	RA	√	√	√	SAR	TD	TD	CM	√
1-Eicosene	3452-07-1 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Docosene	1599-67-3 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Tetracosene	10192-32-2 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
a-olefin fraction C20-24 cut (even numbers)	93924-10-8 Linear	√	RA	RA	RA	RA	RA	√	RA	√	SAR	TD	TD	CM	RA
a-olefin fraction C24-28 cut (even carbon numbers)	93924-11-9 Branched and Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
alkene, C24-54 branched and linear, alpha (even numbers)	131459-42-2 Branched and Linear	√	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA

- √ Adequate existing data available  
 TD Technical discussion provided  
 CM Computer Modeling conducted  
 SAR Structure Activity Relationship (plus measured values where available) provided  
 RA Read-across to existing data for structural analogs (linear alpha olefins and blends of linear and branched internal olefins).