ALFA OLEFINS

CAS N°:592-41-6, 111-66-0, 872-05-9, 112-41-4, 1120-36-1

SIDS Initial Assessment Report
For
11th SIAM

(Orlando, Florida, United States 1/01)

Chemical Name: 1-hexene
CAS No.: 592-41-6

Chemical Name: 1-octene
CAS No.: 111-66-0

Chemical Name: 1-decene
CAS No.: 872-05-9

Chemical Name: 1-dodecene
CAS No.: 112-41-4

Chemical Name: 1-tetradecene
CAS No.: 1120-36-1

Sponsor Country: United States

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HISTORY:

SIDS Dossier and Testing Plan were reviewed at the SIDS Review Meeting or in SIDS Review Process on October 1993. The following SIDS Testing Plan was agreed:

No testing ( )
Testing (x)

Combined reproductive/developmental on 1-hexene, combined repeat dose/reproductive/developmental on 1-tetradecene and acute fish, daphnid and algae on 1-tetradecene.

COMMENTS: The following comments were made at SIAM 6 and have been incorporated in this version of the SIAR:

1. The use of QSAR calculations for aquatic toxicity,
2. More quantitative assessment of effects; and
3. Provide more details for each endpoint.

The following comments were made at SIAM 6, but were not incorporated into the SIAR for the reasons provided:

1. Clarification of the aspiration hazard. The original SIAR stated that C_6-C_{14} alpha olefins were an “animal aspiration hazard”. This statement was based on a reference (Gerarde, 1963) in which rats were anesthetized to induce aspiration because rats are not normally susceptible to such a hazard because they are obligatory nose-breathers. Therefore, the statement has been removed from the SIAR.

2. More quantitative exposure assessments. In order to adhere to the re-focused SIAR format, more quantitative exposure information was only added, if available, from the United States experience and from Finland (for 1-decene only).

Date of Circulation: November 2000
(To all National SIDS Contact Points and the OECD Secretariat)

SIDS INITIAL ASSESSMENT PROFILE

Alfa Olefin Category

CAS No.	592-41-6	111-66-0	872-05-9
Chemical Name	1-hexene	1-octene	1-decene
Structural Formula	CH_2=CH-$(CH_2)_3$-CH_3	CH_2=CH-$(CH_2)_5$-CH_3	CH_2=CH-$(CH_2)_7$-CH_3
CAS No.	112-41-4	1120-36-1	
Chemical Name	1-dodecene	1=tetradecene	
Structural Formula	CH_2=CH-$(CH_2)_9$-CH_3	CH_2=CH-$(CH_2)_{11}$-CH_3	

RECOMMENDATIONS

The chemicals are candidates for further work.

SUMMARY CONCLUSIONS OF THE SIAR

Category Definition

This profile includes an evaluation of SIDS-level testing data, using a category approach, with five individual monoolefins (1-hexene, 1-octene, 1-decene, 1-dodecene, and 1-tetradecene). For the purposes of the OECD SIDS Programme, the category was defined as olefins bearing a single medium-length (C_6 – C_{14}), even-numbered, unbranched aliphatic chain with no other functional groups.

Human Health

Based on screening level tests, all five alpha olefins have been tested and indicate low toxicity concerns for acute oral, dermal and inhalation exposure. These materials are slightly irritating to the skin and eyes of rabbits. In repeated dose studies, 1-hexene, 1-octene and 1-tetradecene have shown comparable levels of low toxicity to female rats (alterations in body and organ weights and changes in certain hematological values) at the higher doses tested (NOAELs of $\geq$ 100 mg/kg oral or $\geq$ 1000 ppm inhalation) and male rat-specific kidney damage that is likely associated with the $alpha_{2u}$-globulin protein (LOAELs $\geq$ 100 mg/kg oral only). Based on screening level testing, they appear not to be neurotoxic (for 1-hexene and 1-tetradecene), produce no adverse effects on reproduction or fetal development (1-hexene and 1-tetradecene), and are not genotoxic (all five of the alpha olefins). As a result, all the above tested endpoints indicate a low hazard potential for human health.

Environment

The potential for exposure of aquatic organisms to C_6-C_{14} alpha olefins will be influenced by their physicochemical properties. The predicted or measured water solubilities of these alpha olefins range from 50 mg/L at 20^0C for 1-hexene to 0.0004 mg/L at 25^0C for 1-tetradecene, which suggests there is a lower potential for exposure to the higher alpha olefins due to their low solubility. Their vapor pressures range from 140 mmHg at 20^0C for 1-hexene to 0.015 mmHg at 25^0C for 1-tetradecene, which suggests the lower alpha olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for longer periods of time.

Several acute aquatic toxicity studies show that 1-hexene and 1-octene have LC/EC50 values below their respective water solubility values (1-hexene: 96 hour LC50 in rainbow trout of 5.6 mg/L and 1-octene: 24 hour EC50 in daphnids of 3.2-10 mg/L). The daphnid value is from an experiment using less than standard exposure conditions (24 hours versus 48 hours). Chronic aquatic toxicity may occur for all of the alpha olefins except 1-tetradecene (predicted 30 day fish toxicity values range from 0.5 to 0.004 mg/L for 1-hexene and 1-dodecene, respectively. Algal toxicity studies were done with all five category members, but the most valid data were with 1-hexene (96 hour EC50 of 22 mg/L). A better understanding of whether these materials are released to water and at what quantities will determine the need to perform chronic aquatic toxicity testing.
Biodegradation data confirm that the C_6-C_{14} alpha olefins degrades in soil and water. They are also expected to degrade in the atmosphere at a rapid rate based on their atmospheric oxidation potentials. Consideration of these degradation processes supports the assessment that these substances will degrade relatively rapidly in the environment and not persist.

Exposure

C_6 – C_{14} Alpha-olefins are major industrial products, which are primarily used as intermediates in the production of the other chemicals and polymers. Other emerging uses are as components of some drilling fluids, and as potential replacements for certain hydrocarbon solvents. Occupational exposures are most likely by the inhalation and dermal routes. Inhalation exposures from industrial manufacture and commercial use are generally considered to be minimal (less than 1 ppm) under normal working conditions. The lower alkenes are minor components of gasoline, or are produced incidentally in combustion of gasoline and polymers, so their presence has been detected in urban air. Such levels were reported to be in the ppb range with a maximum reported value of 0.1 ppm. These alkenes also occur in natural products, although no quantitative values have been reported.

Non-occupational human exposure to alpha olefins is not expected since the compounds are used as industrial intermediates. Atmospheric emissions of alpha olefins from manufacturing are expected to be small and to result primarily from fugitive emission sources originating from compromised hardware (i.e.. faulty seals prior to repair) used in production and storage. On-site waste treatment processes are expected to remove these compounds from aqueous waste streams to the extent that they will not be detectable in effluent discharge. Alpha Olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes. Therefore, environmental exposure to the environment is expected to be minimal.

Category Discussion/Conclusions

A category analysis was done for all the SIDS endpoints by examining available data to determine whether the proposed test plan – to treat the five chemicals as a category – was satisfactory. Results indicate that they were and so no further SIDS-level testing is necessary.

The data indicate an increasing or decreasing trend or pattern from the shortest category member (C_6) to the longest category member (C_{14}) for various physicochemical properties and ecotoxicity (using a mixture of experimental data and estimation techniques), whereas there appears to be no difference across category members for biodegradation and health endpoints.

Melting point, vapor pressure, and water solubility decrease with increasing chain length while boiling point and octano:water partition coefficients increase with increasing chain length. Measured and predicted acute aquatic toxicity data indicate that 1-hexene, 1-octene, and 1-decene exhibit acute effects to aquatic organisms at levels at or below their water solubility; whereas 1-dodecene and 1-tetradecene are not likely to be acutely toxic, probably because they cannot achieve a high enough water concentration to produce acute effects below their water solubility. Predictions of chronic aquatic toxicity suggest that 1-hexene may be less toxic than the rest of the category members and 1-octene, 1-decene, and 1-dodecene are expected to be similarly toxic (estimated values within approximately one order of magnitude among them). The model used (ECOSAR) could not predict the chronic aquatic toxicity of 1-tetradecene. There is no apparent difference regarding biodegradability; available data on four/five category members indicate there are no significant differences among the group. Data presented relative the health effect endpoints of the C_6 – C_{14} alpha olefins indicate no differences among the five category members for acute toxicity, repeat dose toxicity, genotoxicity and reproductive/developmental toxicity.

Given the fact that not all category members were tested for each SIDS endpoint, this analysis shows that where test data exist for more than one category member, it is reasonable to interpolate (and

sometimes extrapolate) for the same endpoint(s) to untested category members. Thus, it is not necessary to test each category member for all SIDS endpoints. It is concluded that using a category approach to evaluate the SIDS-level endpoints for the five alpha-olefins identified above was successful.

NATURE OF FURTHER WORK RECOMMENDED

Further work is recommended in the environmental area. There are no measured data available for chronic toxicity to aquatic organisms, however, computer modelling suggests that 1-octene,1-decene and 1-dodecene may be highly toxic (Chronic value<0.1 mg/L) under chronic exposure conditions. Therefore it is recommended that further data be collected from member countries regarding actual release data from manufacturing and processing facilities to the water compartment at local and national levels. In the event that releases to the water compartment are occurring at levels anticipated to pose a hazard to the aquatic environment, then consideration should be given to determining if chronic aquatic (including sediment-dwelling organisms) toxicity testing would be appropriate.

SIDS INITIAL ASSESSMENT REPORT

Due to the similarities of the C_6-C_{14} alpha olefins, a category approach was utilized to determine the OECD test plan for these compounds. The category is defined as olefins bearing a single, medium length (C_6 – C_{14}), even-numbered, unbranched aliphatic chain with no other functional groups. This SIAR presents testing of "pure substances" and also "blends" of the chemicals as they are produced in their commercial form. For information specific to trends of the category, please see Section 5 of the SIAR entitled, "Category Conclusions".

1. IDENTITY:

The (C_6- C_{14}) alkenes are monoolefins. In general, they are colorless liquids that show decreasing vapor pressure and water solubility with increasing alkyl 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. Table 1A and 1B presents the physical chemical properties of the C_6-C_{14} alpha olefins considered as a category in this assessment.

TABLE 1A: IDENTITY: C_6 to C_{14} ALPHA OLEFINS

Chemical Name	CAS Number	Synonym	Structural Formula
1-HEXENE	592-41-6	Hexene-n-1, C_6 alpha olefin Hex-1-ene	$CH_2=CH(CH_2)_3-CH_3$
1-OCTENE	111-66-0	Octene-n-1, C_8 alpha olefin Oct-1-ene	$CH_3(CH_2)_5CH=CH_2$
1-DECENE	872-05-9	Decene-n-1, Decylene, C_{10} alpha olefin, Dec-1-ene	$CH_2=CH(CH_2)_7CH_3$
1-DODECENE	112-41-4	Dodecene-n-1, Dodecylene C_{12} alpha olefin, Dodec-1-ene	$CH_2=CH(CH_2)_9CH_3$
1-TETRADECENE	1120-36-1	Tetradecene-n-1, Tetradecylene C_{14} alpha olefin, Alpha Tetradecene, Tetradec-1-ene	$CH_2=CH(CH_2)_{11}CH_3$

TABLE 1B: IDENTITY: C_6 to C_{14} ALPHA OLEFINS

Chemical Name	MP (^{0}C)	BP (^{0}C)	VP	Viscosity	Log K_{ow}	WS mg/L	HLC (atm m^3/mol)	K_{oc}
1-HEXENE	-139.8 (ns)	63.3 (ns)	(140 mmHg at 20^{0}C) 186.5 hPa (ns)	0.35 cP/20°C	3.39 (m)	50 @ 20C (c)	0.412 (c)	149(c)
1-OCTENE	-101.7 (ns)	121 – 123 at 1 atm (ns)	(15.2 mmHg) 20.3 hPa at 20^{0}C (m)	0.492 cP/20°C	3.5 – 4.6 (m)	4.1 @ 25C (m)	0.627 (c)	507(c)
1-DECENE	-66 (ns)	172 (ns)	(1.70 mmHg) 2.27 hPa at 20C (ns)	0.75 cP/20°C	>8 (m) 5.4 – 7 (c)	0.115 @ 25C (m)	2.68 (c)	1,724 (c)
1-DODECENE	-35 (m)	214 at 20^{0}C at 101.3 kPa (ns)	1.6x10^{-1} mmHg at 25C, 0.21 hPa (ns)	1.18 cP/20°C	>8 (m) 6.1 (c)	0.113 (c)	4.25 (c)	5,864 (c)
1-TETRADECENE	-12 (ns)	252 at 1 atm (ns)	1.5x10^{-2} mmHg at 25C, 0.02 hPa (m)	4.4 cP/20°C	7.08 (c)	0.0004 @ 25C (c)	8.48 (c)	19,950 (c)

Calculated (c) by EPIWIN, Measured (m) and Not specified (ns)

2. GENERAL INFORMATION ON EXPOSURE

A. Production Volume

a. Manufacturing

The major commercial processes used in the production of linear olefins are the cracking of petrochemical waxes, and oligomerization of ethylene using the Ziegler process, or a modern modification of it (Demianiw, 1981). They may also be made as a byproduct from the liquefaction of coal. In the past, linear olefins were produced by the chlorination-dechlorination of linear alkanes; however, it is likely that this process is no longer used on a commercial basis. The ethylene oligomerization process can produce better-defined mixtures limited to even-numbered carbon chains, yet rich in terminal (alpha) olefins. Product distribution can be controlled by adjusting the process parameters and by the choice of catalyst.

Current United States aggregate production ranges as of 1998 for all members of the (C6-C14) alkenes are 100 – 500 million pounds (45,360 – 226,800 tonnes). When looking at previous production ranges dated from 1986 there does appear to be an increase in production for dodecene and tetradecene from 1-100 million pounds (453.6 tonnes – 45,360 tonnes) to 100-500 million pounds (45,360 – 226,800 tonnes). Only aggregate production ranges are available in order to mask any confidential business information and are based on production volumes reported in the USEPA IUR.

The production volume of 1-decene in Europe for 1999 is reported to be around 100,000 tons and the volume for the processing of 1-decene as an intermediate in the production of other chemicals, in Europe for 1999, is estimated to be 160,000 tons. (Nikunen and Heiskanen, 2000)

b. Inadvertent Production

Inadvertent production of individual components of the (C_6-C_{14}) alkenes reportedly occurs from the thermal destruction of some petroleum-based products. 1-Hexene, 1-decene and 1-dodecene are not manufactured by the petroleum industry as discrete products, but are present in naptha and light distillate intermediate refinery process streams due to incidental production during catalytic cracking and pyrolysis. Concentrations of these compounds in petroleum process streams and in finished products range from less than 1 to 10% (volume basis) and 0 to 3.6% (volume basis), respectively. Levels in aviation gasoline and diesel fuels have been estimated to be one-tenth those in automotive gasoline. (CRCS Inc., 1985).

B. Uses and Functions

Linear alpha olefins are utilized as intermediates in the manufacture of a number of products: oxo alcohols, alkyldimethylamines, surfactants (e.g., alpha olefin sulfonates), plastics (e.g., high density and linear low density polyethylenes) and synthetic fatty acids, lube oil additives, linear mercaptans, alkenylsuccinic anhydrides, epoxides, and leather treating compounds (CMR, 1988; CRCS, 1985; Demianiw, 1981). As of this writing, the use pattern has not appeared to change. Listed in Table 2 are the applications of the (C_6 – C_{12}) alpha olefins along with alpha olefin mixtures as indicated by Ethyl (1984), Chevron (1984) and CRCS (1985) with the exception of data obtained for tetradecene. Uses for tetradecene were obtained from the dossier.

TABLE 2: (C_6-C_{14}) Alpha Olefin Uses

	Individual Chemicals				BLENDS					
Primary Applications	C_6	C_8[4&5]	C_{10}	C_{12}	C_{14}	C_6-C_7	C_6-C_9	C_8-C_9	C_8-C_{10}	C_{11}-C_{12}
Comonomer in polyethylene	X	X	X							
OXO alcohol intermediate	X	X	X	X	X[1]	X		X		X
Synthetic fatty acid intermediate	X	X	X							
Synthetic lubricant intermediate			X		X[1]		X	X	X	
Alkylbenzene feedstock		X	X	X				X	X	
Epoxide intermediate		X	X							
Amine, amine oxide, and mercaptan intermediate			X	X	X[1]					
Metal working and gear oil additive			X							
Dielectric Fluids[2]								X[2]		
Processing as intermediate in production of other chemicals[4]			X							
Intermediate in the manufacture of alkyl succinic anhydrides, mercaptans, alkyl silanes, polyol esters[5]		X								

[1](Dossier, tetradecene)
[2](Baarschers, 1983)
[3](Nikunen and Heiskanen, 2000)
[4]American Chemistry Council, comments from Spolana, 2000)
[5]per Chevron Phillips Chemical Company

Some olefins are being investigated as replacements for hydrocarbon solvents of higher volatility, and as components of inert drilling fluids for oil exploration and production (Chevron-personal communication).

C. Sources of Release to the Environment

a. Production Releases

Chevron (1984) reported that atmospheric emissions of alpha olefins from manufacturing are expected to be small. However, the EPA (1977) noted that olefins might be released to the atmosphere in small quantities due to leaks in process equipment used during production of the compounds. It is likely that the alpha olefins are released in aqueous effluents and atmospheric emissions from manufacturing, use operations and from fuel processing and combustion. (CRCS, 1985)

b. Other Releases to the Environment:

(a)Releases from by-products other than industrial: 1-Hexene has been identified in the gases produced during structural fires and in the field-burning of agricultural plastic (Lowery et al., 1985 and Linak et al., 1989). The commercial liquefaction of coal by the solvent refining process can produce hexene and other olefins, along with the desired hydrocarbon products (Wright et al., 1984). 1-Hexene has been identified in the exhaust of roadway vehicles (Sigsby et al., 1987; Stump and Dropkin, 1985).

Hexene and octene have been identified as products of combustion of polyethylene (Hodgkin et al., 1982). 1-Hexene, 1-octene and 1-decene, have been identified in the emission of high-altitude jet aircraft engines (Katzman and Libby, 1975).

1-Hexene was detected in the air of a high-volume gasoline service station, at concentrations of up to 0.1 ppm (Kearney and Dunham, 1986). C_6 Olefins (isomers unspecified) were reported to comprise 1.8% of gasoline (ATSDR, 1993).

(b) Natural Occurrence: API (1985) reported that 1-hexene, 1-decene and 1-dodecene probably do not occur naturally in crude oils. Some specific isomers of the (C_6-C_{14}) alkenes have been identified as naturally occurring compounds.

1-Hexene was identified as a product of the microbial breakdown of the natural terpene b-carotene (Hunt et al., 1980).

1-Octene has been identified as a major volatile constituent of irradiated fresh chicken (Hansen et al., 1987).

1-Decene has been isolated from the leaves and rhizome of the plant *Farfugium japonicum* (Kurihara and Suzuki, 1980). 1-Decene has been detected as the initial product in the microbial degradation of n-decane (Iida and Iizuka, 1970).

2.1 ENVIRONMENTAL EXPOSURE AND FATE

A. General Discussion: Information from production, use and physicochemical properties (Described in section 2) suggests that C_6-C_{14} alpha olefins (AOs) have the potential to partition to various compartments of the environment. However, releases to the environment are likely to be largely to the air, followed by surface waters, from manufacturing practices, combustion and natural production. In the atmosphere, -OH radicals can rapidly degrade AOs. They have also been shown to be biodegradable, which suggests they have a potential to be biodegraded in water, as well as soil and sediment. As a result, potential for exposure to AOs in the environment should be low and they are not expected to persist. An environmental exposure analysis for 1-decene in the aquatic and terrestrial compartment has been performed by Finland and is located in Appendix A.

A summary of environmental fate data is found in Table 3. When measured data were not available, computer models were utilized to estimate environmental fate and distribution. Information on the computer models is provided in Appendix B of the SIAR. Model input values along with results may be found in the individual chemical's SIDS dossier.

B. Photodegradation: In the air, all the AOs are subject to atmospheric oxidation from hydroxyl radical (-OH) attack. Their atmospheric oxidation rates can be determined (EPIWIN, 1999) based on structure. The AOs are calculated to have half-lives ranging between 3.3 to 9.3 hours, which suggests that once volatilized to the air, these chemicals will degrade rapidly (Table 3).

C. Waste Water Treatment Plant (WWTP): Although AOs may be found in effluent from waste water treatment plants (WWTPs) receiving influent from AO manufacturing, use and fuel processing operations, the primary mode of disposal of these chemicals is incineration or diversion to other hydrocarbon uses (recycling). The overall removal rate of the AOs entering a WWTP with secondary treatment is calculated (via EPIWIN modeling) to be >99% for the $C_6 - C_{10}$ molecules and >90% for the C_{12}-C_{14} molecules. Because they have relatively high vapor pressures and/or high Henry's Law constants (Table 1B), volatilization can be a major contributing factor in the removal of AOs from influent in WWTPs with aerated secondary treatment. Another route of AO loss from a WWTP can result from sorption processes (see section D.c below). Sorption of the higher chain AOs to solids may be a significant loss process as solids are separated during treatment and removed for further disposal. AOs have also been shown to biodegrade at a significant rate (see E below and Table 3). This suggests that the fraction of non-volatilized material remaining in a WWTP is subject to biodegradation, which can further decrease AO concentrations in treatment plant influent.

D. Distribution in Air, Water and Soil

a. ***Distribution utilizing a fugacity level I model***: A Level I fugacity model calculates the distribution of a chemical under steady state, equilibrium conditions throughout a defined generic environment. Level I calculations do not consider chemical degradation, advection, or intermedia transport processes. The level I environment is a closed system, referred to as a "unit world", which contains six environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota) with fixed volumes. A chemical's distribution in the level I environment is based only on selected physical parameters of the chemical being modeled. The results show the percent distribution of a chemical among the six environmental compartments.

b. ***Distribution using a level III fugacity model***: A Level III fugacity model calculates the distribution of a chemical under steady state, non equilibrium conditions, 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 do 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. To represent actual emission rates from a production facility, a ratio of 10:1:0 for air, water and soil was used (based on estimated ratios from the American Chemisty Council, 2000). Percent distribution results using the emission values from the American Chemistry Council are presented in Table 3. A comparison of the distribution data utilizing the default values and the values provided by the American Chemistry Council are presented in Appendix B.

Results of the modeling using the estimated emission assumptions from the American Chemistry Council suggest that the water compartment is the primary environmental compartment to which C6 and C8 AOs will partition. As the chain length increases beyond C8, sediment becomes the primary compartment followed by the water and then air. The greater affinity of the higher molecular weight AOs to partition to sediment is supported by their high Koc partition coefficients.

This can be attributed to the AO having a high tendency to bind to particulate matter in the water column thus binding more to soil and sediment. The high organic/carbon partition coefficient (Koc) of this chemical class supports this type of partitioning. The longer the AOs are in chain length, the less likely they are to partition to the atmosphere and water.

c. Sorption to soil and sediment: The potential of a chemical to sorb to soil and sediment can be indicated by its Koc value. The lower the Koc value, the lower the tendency of a chemical to sorb to the organic matter contained by the soil or sediment. Modeled Koc values for the AOs are as follows: C_6=149, C_8=507, C_{10}=1,724, C_{12}=5,864 and C_{14}=19,950. These data in conjunction with the information referenced in Table 3 suggest that the C_6 to C_8 AOs are expected to exhibit low to moderate sorption, respectively, while the remaining olefins up to C_{14} will demonstrate an increasingly greater tendency to sorb to organic matter. These data also relate to the potential of these chemicals to migrate through soil and sediment.

d. *Migration to ground water*: Swann et al. (1983) reported that a chemical with a Koc value between 150 and 500 would move through the soil at a moderate rate. This rate slows between 500 and 2,000. Chemicals with Koc 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 Koc

data indicate that the lower chain AOs, C_6-C_8, show 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 a C_{14} olefin has only a negligible, if any, potential for migration. These are general characterizations based on the Koc values for these chemicals, which with increasing carbon number show that there is an increasing tendency to sorb to organic matter (see c. above). 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.

E. Abiotic and Biotic Degradation: Measured and modeled data (Table 3) suggest that the AOs have the potential to biodegrade at a relatively rapid rate.

A number of studies have been reported with 1-hexene. Shell Research Limited, (1985) showed that "Shop C6 Alpha Olefins" had an observed 22% of theoretical oxygen demand in 28 days in a Closed Bottle test. The same report states that 1-hexene was not readily biodegradable in a modified STURM test. MITI, (1992) used an Organization of Economic and Co-operative Development (OECD) test guideline, which showed a range of biodegradation, from 67 to 98% in 28 days (as BOD). The MITI study is considered more appropriate for use in this analysis because the Shell studies appear to use a mixture (rather than pure 1-hexene; as was apparently used in the MITI study) and also because hexene is volatile and the modified STURM test is not an appropriate protocol for the volatile substances.

Similarly, there are a variety of biodegradation studies reported in the individual dossiers in which mixtures were apparently used. For the purposes of this report, results with pure compounds were considered more relevant. Biodegradation studies with 1-octene, 1-decene, and 1-tetradecene showed degradation rates of 41-42% after 28 days (Adema and Bakker, 1985); 81% after 28 days (Enichem Instituto G Donegani, 1995); and 45-65% (Turner, 1985), respectively. Thus, there is no apparent difference regarding biodegradability; available data on four/five category members indicate there are no significant differences among the group.

F.Volatilization: In general, volatilization of the AOs to the air could occur at relatively rapid rates depending on environmental factors (i.e., surface type, temperature, wind velocity) and the compartment from which volatilization is being considered (i.e., soil, water). The volatilization of the lower chain AOs in comparison to the higher chain AOs will be more significant from soil, while the volatilization of all the AOs under discussion could be significant from water. The latter is true for the higher chain AOs as well, based on their Henry's Law constants (HLC) (Table 1B). As a HLC increases, there is a greater tendency of the chemical to volatilize from water. All of the AOs have HLCs in a range that suggests they will volatilize from water at a rapid rate (Lyman, 1990).

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 mmHg, suggesting that they will tend to volatize from surface soils at a relatively rapid rate. In comparison the C_{12}-C_{14} olefins have vapor pressures less than 1 mmHg, 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 (see section E. above) because they have a lower potential to migrate and volatilize.

TABLE 3: Environmental Fate and Transport of the C_6-C_{14} Alpha Olefins

	WWTP % removal	Distribution fugacity level III*	Distribution fugacity level I	Migration to groundwater (EAB-IRER, 97)	Sorption to soil and sediment	Biodegradation	Atmospheric oxidation $T_{1/2}$	Volatilization from water $T_{1/2}$	Volatilization from soil
Hexene	>99	Air = 21 Water= 77 Soil= <1 Sediment= 2	Air = 100 Water= <1 Soil=<1 Sediment=<1	Moderate to rapid; may be mitigated by volatilization	Low to moderate (EAB-IRER, 1995)	67 – 98% after 28 days (m) (MITI, 1991) Volatilization is expected to be more rapid than biodegradation (EAB-IRER, 1996)	-OH = 4.2 hrs O_3 = 23 hrs (EPIWIN, 99)	River = 0.9 hrs Lake = 4 days (EPIWIN, 96)	Moderate mobility Dry Soil: May exist Moist Soil: Rapidly (Swann et al 1983; and EPIWIN, 1999)
Octene	>99	Air = 15 Water= 61 Soil= <1 Sediment= 23	Air = 99.7 Water= <1 Soil=<1 Sediment=<1	Moderate; may be mitigated by volatilization	Moderate (EAB-IRER, 1997)	41-42% after 28 days (m)(Adema and Bakker, 1985) Volatilization is expected to be more rapid than biodegradation (EAB-IRER, 1996)	-OH = 3.8 hrs O_3 = 22 hrs (EPIWIN, 99)	River = 1 hrs Lake = 4 days (EPIWIN, 96)	Moderate mobility Dry Soil: May exist Moist Soil: Rapidly (Swann et al 1983; and EPIWIN, 1999)
Decene	>99	Air = 5 Water= 19 Soil= <1 Sediment= 76	Air = 99.2 Water= <1 Soil=<1 Sediment=<1	Slow; may be mitigated by rapid volatilization	Strong (EAB-IRER, 1997)	81% after 28 days (m) (Enichem Institute G Donegani, 1995) Aerobic: days to weeks Anaerobic: weeks to months	-OH = 3.6 hrs O_3 = 22.9 hrs (EPIWIN, 99)	River = 1.2 hrs Lake = 5 days (EPIWIN, 96)	Low mobility Dry Soil: May exist Moist Soil: Rapidly (Swann et al 1983); EPIWIN, 1999
Dodecene	>90	Air = 3 Water= 12 Soil= <1 Sediment= 85	Air = 84.9 Water= <1 Soil=14.7 Sediment=<1	Negligible	Strong (HSDB, 1996; EAB-IRER, 1997)	Aerobic: weeks	-OH = 3.3 hrs O_3 = 22.9 hrs (EPIWIN, 99)	River = 3.8 hrs Pond = 17 months (HSDB, 96)	Slight mobility Dry Soil: Slowly Moist Soil: Rapid (HSDB, 96; Swann et al. 1983 and EPIWIN, 1999) It is expected that strong sorption may attenuate this process.
Tetradecene	>90	Air = 5 Water= 6 Soil= <1 Sediment= 89	Air = 94.9 Water= <1 Soil=5 Sediment=<1	Negligible	Strong (HSDB, 1996)	48-64% after 28 days (Turner, 1985) (m) Aerobic: weeks	-OH = 9.3 hrs O_3 = 23 hrs (HSDB, 96)	River = 4.1 hrs Pond = 7.3 months (HSDB, 96)	Immobile Dry Soil: Will not volatize Moist Soil: Rapidly (HSDB, 96; Swann etal., 1983, EPIWIN, 1999) It is expected that strong sorption may attenuate this process.

All values calculated via EPIWIN,99 unless otherwise noted except for fugacity modeling which utilized the EQC model.
(m) = measured value
*Based on the following emission rates: 10 kg/hr to air, 1 kg/hr to water, 0 kg/hr to soil.

2.2 Human Exposure

A. Occupational Exposure: Occupational exposure to the (C_6-C_{14}) alkenes is most likely to occur through dermal contact and inhalation during the production, formulation, transportation, or use of these compounds. No data on occupational exposure from the direct use of the (C_6-C_{14}) alkenes were located in the open literature.

Occupational exposure limits for (C_6-C_{14}) alkenes have not been established by the Occupational Safety and Health Administration (OSHA). The American Conference of Governmental Industrial Hygienists (ACGIH) has recently proposed a change (from 30 ppm (103 mg/m^3) to 50 ppm (172 mg/m3) in the threshold limit value (TLV) for 1-hexene (ACGIH, 2001). Workplace exposure data on these compounds gathered by the National Institute of Occupational Safety and Health (NIOSH) in the National Occupational Exposure Survey (NOES) are shown below:

- 1-hexene: 7974 workers in 8 SIC code industries;
- 1-dodecene: 300 workers, including 4 females, in 1 SIC code industry

Shell reported that their internal standard for worker exposure to 1-hexene, 1-octene and 1-decene is 100 ppm TWA (344 mg/m^3, 458 mg/m^3, 572 mg/m^3), respectively. Phillips detected an 8-hr TWA exposure level of 0.12 ppm (0.413 mg/m^3) for 1-hexene in their plant based on a monitoring survey involving 59 measurements. Chevron and Ethyl reported that closed systems are used in the manufacture and use of alpha olefins. Chevron and Ethyl reported that exposure is confined to reactor operators, maintenance personnel, and personnel involved in loading and off-loading of tank trucks or cars. Exposure levels are anticipated to be below 1 ppm during normal operating conditions.

The American Petroleum Institute reported that the intermediate refinery process streams that contain (C_6-C_{14}) alkenes are processed in closed systems, presenting minimal opportunity for worker exposure at the refinery.

Occupational exposure to the (C_6-C_{14}) alkenes can also occur from their presence in work-related media. 1-Hexene was detected in the air of a high-volume gasoline service station, at concentrations of up to 0.1 ppm (0.34 mg/m^3) (Kearney and Dunham, 1986). C_6 Olefins [isomers unspecified] were reported to comprise 1.8% of gasoline [ATSDR, 1993]. The mean personal air concentrations of 1-hexene arising from gasoline for workers in the petroleum industry were 0.019 mg/m^3 (0.006 ppm) for outside operators, 0.088 mg/m^3 (0.03 ppm) for transport drivers, and 0.281 mg/m^3 (0.08 ppm) for service attendants (Rappaport et al., 1987).

Hexenes, octenes, and decenes were detected in air samples taken from landfills in the United Kingdom, including municipal, industrial, and liquid co-disposal sites (Young and Parker, 1984). Octene has been detected in air samples taken at a water treatment plant in Switzerland [Hangartner, 1979].

B.Consumer Exposure: There are no reports of exposure from the use of alpha olefins in consumer products. Non-occupational human exposure to alpha olefins is not expected since the compounds are used as industrial intermediates (CRCS, 1985). According to Finland (2000) consumer exposure may occur during the usage of self-service gasoline stations, which may lead to indirect exposures of individuals living in close proximity to the self-service gasoline station.

C. Indirect Exposure Via the Environment: General population exposure to (C_6- C_{12}) alkenes is probably limited to contact with low concentration of the compounds in ambient air and finished petroleum products.

Exposure to the general population may occur during use of petrochemical products that contain the linear olefins. Inhalation exposure to 1-hexene may occur for those who use self-service gas stations (Kearney and Dunham, 1986).

Exposure of the general population to the (C_6-C_{14}) alkenes may occur through the ingestion of contaminated food. 1-Decene and 1-dodecene have been identified in walleye and trout taken from the Great Lakes (Hesselberg and Seelye, 1982). Octene has been detected in oysters and clams obtained from Lake Pontchartrain, LA (Ferrario et al., 1982).

D. Drinking Water Exposure: Exposure of the general population to (C_6-C_{14}) alkenes may occur by ingestion of drinking water (Lucas et al., 1984). 1-Hexene, 1-octene, 1-decene, and 1-dodecene have been identified in drinking water samples from the United Kingdom (Fielding et al., 1981) but levels were not reported.

3. HUMAN HEALTH

The exposure routes of concern for human health are considered to be dermal and inhalation. Data presented in the SIAR are considered the key studies to describe the hazard of these compounds. All other data may be found in each individual chemicals respective dossier. A summary of all data presented in the SIAR may be found in Table 4.

3.1 Effects on Human Health

A. Acute Toxicity: By oral and dermal routes in rats and rabbits, respectively, the median lethal dose values (LD50) are greater than 10 g/kg for all five AO compounds. By the inhalation route in rats and mice results indicate that there does not appear to be a concern for acute toxicity with all five of the AO compounds.

B. Irritation: Under semi-occluded conditions, C_6- C_{14} alpha olefins appear to be mildly irritating to rabbit skin when tested as pure chemicals (range of mean primary irritation scores [based on 0- 8.0] was 0.1 for 1-dodecene to1.8 for 1-octene); but appear to be slightly to severely irritating when tested as blends or mixtures (primary irritation scores of 3.38 for NEODENE 8, 4.3-5.1 for Alpha Olefin PQ11 103, 4.67 for Gulftene 12, and 4.5 for NEODENE 14). The alpha-olefins appear to be only slightly irritating to rabbit eyes, regardless of whether the test material was pure or a mixture (range of mean Draize scores [based on 0 - 110] was 0.0 for 1-decene and Alpha Olefin PQ11 103, 4.7 for NEODENE 8). The alpha olefins do not cause skin sensitization in guinea pigs.

C. Repeated Dose Toxicity: In studies with animals, C_6- C_{14} alpha olefins have demonstrated a low level of toxicity following repeated exposures using the oral, inhalation, and dermal routes.

a. Oral studies:

1-hexene: Groups of 5 male and female rats were exposed to 1-hexene via gavage for 28 days at 10, 101, 1010 and 3365 mg/kg/day (Dotti et al., 1994). The main effect exhibited was irritation of the gastric mucosa at the two top dose levels (males and females) along with reduced body weights (at the top two dose levels in males and the top dose only in females). Spleen weights were reduced at the top dose of 3365 mg/kg/day in males, 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.

Gingell et al (2000) conducted a combined reproductive/developmental toxicity study 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.F. Male rats were dosed for 44 consecutive days and the following kidney effects were observed: 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 convulted tubules in all treated rats (incidence of 0/0, 7/12, 8/12 and 9/12 for the 0, 100, 500 and 1000 mg/kg/day). The extent of hyaline droplet formation also increased with dose. Although there was no immunochemical verification, the author's concluded that the formed droplets were alpha2u-globulin.

1-octene: Four groups of 20 male and female rats were dosed via gavage with 1-octene for 90 days at 0 (control), 5, 50, and 500 mg/kg/day. Changes 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) and decreased plasma chloride (in both sexes), increased plasma creatinine concentration (females only). These findings indicate a nephrotoxic effect at 500 mg/kg/day. The author 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 author's 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 was no significant difference 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.

1-tetradecene: Rats were orally dosed with 1-tetradecene (OECD modified 422) at concentrations of 100, 500, and 1000 mg/kg/day. (The test protocol and reproductive/ developmental toxicity results from this study are discussed in section 3.F. below). The neurotoxicity option in the test protocol was followed and showed no effects in males or females at any dose level. It was observed that hepatocyte cytoplasmic vacuolation occurred in both sexes at $\geq$500 mg/kg/day (associated with an increase in liver weight), and pitted kidneys and accumulation of hyaline droplets in the proximal convoluted tubules of the kidneys of males at all dose levels. The kidney effects were interpreted to be a result of hydrocarbon nephropathy, which is specific to male rats. The determined NOEL was 100 mg/kg/day (the effect was liver effects in non-pregnant satellite females histologically examined). A NOEL for systemic toxicity to the males was not determined due to the hydrocarbon nephropathy.

b. 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, 1999; on Shell, 1984). Rats were exposed to 0, 300, 1000, and 3000 ppm 1-hexene for 90 days (6 hrs/day, 5 days/week) and evaluated for systemic toxicity. No mortalities and no treatment-related clinical signs of toxicity were seen. At 3000 ppm, females had significantly lower body weights. Slight but statistically significant clinical pathological changes which may have been treatment-related included: elevated serum phosphorus in males at 300, 1000, and 3000 ppm and in female rats 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; and lower mean corpuscular hemoglobin and hemoglobin concentration in 1000 and 3000 ppm females. At 3000 ppm, males had statistically higher relative and absolute testes weights; however, when the left testicle was detunicated prior to weighing, there was no statistically significant increase in testis weight compared with the controls. No treatment-related gross or histological lesions were noted in these or other tissues. The NOAEL appeared to be 1000 ppm, based on changes in body weight and questionable organ weight changes at 3000 ppm.

c. Dermal:

Two dermal studies were conducted, one with rats (2 week study with a C_{12}-C_{16} blend) and one with rabbits (28 day study with C_8). The rabbit study was a 28-day irritation study in which animals were treated with 0.2 ml of the test substance 5 days/wk for four weeks (Ethyl Corporation, 1973). Results showed "questionable hyperemia, exfoliation, and scab formation". There was no assessment for systemic effects and only one dose was used. In rats, repeated dermal application of a C_{12}-C_{16} blend for two weeks at 0, 1, or 2 g/kg resulted in severe skin reactions and depresses body

weights only at the highest dose tested (Gulf Life Sciences 1983). No other treatment related effects were noted.

D. Genetic Toxicity: The C_6-C_{14} alpha olefins are not considered to be genotoxic as a result of a broad range of *in vitro* studies (bacterial reverse mutation; mitotic gene conversion in yeast; mammalian cell gene mutation, chromosome aberration, and transformation; and unscheduled DNA synthesis). Negative results were also seen *in vivo* in bone marrow micronucleus tests in which mice were exposed via inhalation to 1000 - 25,000 ppm 1-hexene for 2 hrs/day for 2 days. Dermal application of a C_{12}-C_{16} blend of alpha olefins to mice also failed to induce an increase in micronucleated bone marrow erythrocytes.

E. Toxicodynamics, toxico-kinetics: Studies with C_6, C_8, C_{10}, and C_{12} alpha olefins indicate that metabolism occurs in hepatic endoplasmic reticulum via initial formation of a transient epoxide which are further metabolized to the corresponding glycol or conjugated with glutathione. The latter two metabolites are excreted in urine as mercapturic acids. (Watabe, 1968; Maynert, 1970; Oesch, 1973; Sipes, 1991).

1-Hexene was included in a study to determine the ability of 1-alkenes to form epoxides by the presence of hemoglobin and DNA adduct formation in the blood of rats exposed via inhalation (Eide et al., 1995). Results showed a decrease in hemoglobin and DNA adduct formation with an increase in 1-alkene chain length (the study included C2-C8 alkenes).

F. Reproductive/Developmental Toxicity: Two separate studies are reported here: a combined reproductive/developmental study with 1-hexene and a combined reproductive/ developmental study with tetradecene.

1-Hexene was orally administered via gavage to male and female rats in a combined reproductive/developmental toxicity test (OECD 421) at the following doses: 0, 100, 500 and 1000 mg/kg/day in corn oil (Gingell et al., 2000 on EM Daniel, 1995). 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 developmental toxicity parameters: number of litters, pup survival, pup viability, pup weight, and sex ratio. There were no effects on the following reproductive parameters: precoital intervals, gestation length, pregnancy rats, 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, no evidence of impared fertility in the treated males and there was a lack of a dose response between treated groups. . Therefore, the NOAEL for reproductive/developmental toxicity is 1000 mg/kg/day. The kidney effects observed in F0 males have been described previously in section 3.1.C.a.

1-tetradecene, administered orally, was evaluated for reproductive and developmental toxicity in a combined repeat dose/reproductive/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). A satellite group of eight females were assessed for neurotoxic and pathological analyses(see section 3.G.b). 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. There was no

evidence of developmental toxicity in the F1 generation, as measured by 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 reproductive/developmental effects was >1000 mg/kg/day.

G. Other:

a) Carcinogenicity: No carcinogenicity tests have been conducted on C_6-C_{14} alpha olefins. However, there are no structural alerts indicating a potential for carcinogenicity.

b) Neurotoxicity: Neurotoxicity was evaluated in three studies as part of other test protocols already discussed above, two performed with hexene (Neodene 6) and the other with tetradecene. 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 by administration orally for 28 days (3365 mg/kg/day) or via inhalation for 90 days (3000 ppm). 1-tetradecene was tested in a combined repeat dose/reproductive/developmental toxicity screen, which evaluated a satellite group of eight females motor activity, clinical pathology and functional observational battery of rats. Results indicated that there were no test article-related differences that would indicate neurotoxicity in rats treated orally at 1000 mg/kg/day.

c) Observations in Humans: In a review, Cavender (1993) noted that 1-hexene, when inhaled, at a concentration of 0.1 percent (1000 ppm), causes CNS depression with mucous membrane irritation, vertigo, vomiting and cyanosis. When ingested it presents a moderate aspiration hazard.

Chevron (1984) reported that prolonged or frequently repeated contact with (C_6 – C_{12}) alkenes might cause the skin to become dry or cracked from the defatting action of the compounds. Breathing of vapor of (C_6 – C_{12}) alkenes may cause CNS depression. Signs and symptoms of CNS depression may include one or more of the following: headache, dizziness, and loss of appetite, weakness and loss of coordination. Affected persons usually experience complete recovery when removed from the exposure area.

Table 4: Health Effects of the C6-C14 Alpha Olefins

	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
Hexene	Oral: Rat LD50>5600 mg/kg and >10,000 mg/kg Inhalation: Rat LC50 (4hr) = 32,000 ppm (nom)	Rat, 90-day inhalation OECD 413; NOEL= 1000 ppm[1] Rat, 28-day gavage OECD 407; NOEL=101 mg/kg (gastric effects [males and females] and reduced body weights [males only]) Rat; OECD 421; NOEL ≥100 mg/kg (general tox –male rat nephropathy);	*S. typhimurium*, OECD 471 w/out repeat assay; Mouse Lymphoma, OECD 476, ; Mammalian Cell gene mutation ; CHO, OECD 473, Human lymphocytes-Metaphase Chromosome Analysis. All negative with and w/out activation— UDS-rat hepatocyte; OECD 482; Negative at 0.5 and 2 mg/ml; no evaluation at 3.5 and 5.0 mg/mL due to toxicity. BALB/3T3 cells transformation-Negative	Mouse Bone Marrow micronucleus; Mouse; OECD 474 (inhln); Negative at 0, 1000, 10000 and 25000 ppm	Rat; OECD 421; doses at 0, 100, 500, and 1000. NOEL=>1000 mg/kg (reproductive tox, parental, adult female); NOEL =>1000mg.kg (reproductive tox, F1 generation); NOEL=>1000 mg/kg (Pregnancy litter); NOEL=>1000 mg/kg (foetal data)[2]
Octene	Oral: Rat LD50>10g/kg and >5 ml/kg Inhalation: Rat LC50 (4 hr) = 8,050 ppm (nom) Dermal: Rabbit LD50 >10 g/kg (24 hr) and 1.43 g/kg (24 hr)	Rat, 90 day oral (gavage) dosing at 0,5,50 or 500 mg/kg/bw – NOEL = 50 mg/kg/day increased kidney weights and decreased plasma chloride in both sexes Rabbit 28-day dermal irritation study at 0.2 ml, 5 days/week for 4 weeks. Questionable hyperemia, exfoliation, and scab formation.	*S.typhimurium*; Neodene 8, *S.typhimurium*; Octene and BALB/c-3T3 transformation: Negative with and w/out activation Two CHO chromosome abberrations 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.		
Decene	Oral: Rat LD50>10g/kg Inhalation: Rat LC50 >saturation conc for 1 and 4 hr exposure at saturation of 9.3 and 8.7 mg/L		*S.typhimurium*; OECD 471; Negative with and w/out activation		
Dodecene	Oral: Rat LD50>7.7 g/kg, >10 g/kg and >10g/kg Inhalation: Rat LC50 (4 hr) > 2.1 mg/l; (1hr) >9.9 mg/L	Rat 2-week dermal toxicity at 0, 1, or 2 g/kg C12-C16 blend. Severe skin reactions and depressed body weights at 2g/kg.	*S. typhimurium* and *E.coli*; Blend[3] and C12 and CHO/HGPRT; Blend[3], Mitotic Gene conversion Assay; *S. cerevisiae*; Blend[3] and C12: All negative with and w/out activation CA; Rat liver; RL1 cells; C12, CA; Rat liver, RL4 cells; Blend[3], BALB/3T3 Mouse embryo; Blend[3] and UDS; Blend[3]: All negative	Mouse Micronucleus Bone Marrow Test (dermal); Blend; No remarkable clinical findings-negative at dose of 5000 mg/kg (only dose admin)	

Tetradecene	Oral: Rat LD50 17.3 g/kg and >10g/kg; Mouse LD50= 21.3 g/kg Inhalation: Rat LC50 (1hr) = 9900 mg/m^3 Inhalation: Mouse LC50 = 223 mg/L	Combined OECD 422; gavage dosing at 0, 100, 500 or 1000 mg/kg/bw/day for up to 51 days. NOAEL = 100 mg/kg/day liver effects in non-pregnant female satellite group and no NOEL for males due to kidney effects Rat 2-week dermal toxicity at 0, 1, or 2 g/kg C12-C16 blend. Severe skin reactions and depressed body weights at 2g/kg.	*S. typhimurium*; Blend[3], Mitotic recombination; *S. cervisiae*; Blend[3], Rat Liver RL1 cells; Blend[3], and CHO cells; Blend[3]: Negative with and w/out activation UDS; rat hepatocyte; Blend[3], and BALB/c-3T3; Blend[3]: Negative	Mouse Micronucleus Assay (dermal); Blend; Negative at doses of 1000; 2500 and 5000 mg/kg for 2 days.	Rat; Modified OECD 422; gavage at 0.100,500 or 1000 mg/kg/bw/day for up to 51 days; NOAEL parental: 1000 mg/kg/bw/day; NOAEL F1 Offspring; 1000 mg/kg/day No developmental effects seen through day 4 of lactation

[1]Neodene 6 = 90-100% hexene;
[2]Three test articles blended to produce final test article consisting of 90-100% hexene.
[3]Blend not specified.

4. Effects on the Environment

4.1 Aquatic Effects

Table 5A summarizes the acute aquatic toxicity data (both experimental and modeled) and Table 5B presents the results of modeling the chronic toxicity of the alpha olefin category members. The Daphnid and fish acute toxicity studies were conducted with relatively pure alpha olefins except for the test material used in the 1-decene and 1-dodecene experiment, which was a blend of olefins ranging in carbon number from C_{10}-C_{13}. The results for a test material with a mixture of olefins ranging from a C_6 to a C_8 are used to characterize the algal toxicity of 1-octene. The algal studies for 1-hexene and 1-tetradecene were conducted using relatively pure chemicals. In many cases, the concentrations tested were much greater than the water solubility of the test substance.

No chronic toxicity data were found. Because of the limited amount of measured acute data an aquatic toxicity computer model (ECOSAR) was used to estimate algal toxicity and acute toxicity to Daphnids and fish to support the existing measured data. This model was also used to estimate a chronic value for fish because of the lack of measured data. Information concerning the basis for the computer models can be found in the Appendix B of the SIAR. Model input values along with results may be found in each individual chemical's respective SIDS dossier.

A. Acute Toxicity

a. 1-Hexene: Toxicity data are available for an alga (*Selenastrum capricornutum*), Daphnid (*Daphnia magna*), and two fish, rainbow trout (*Salmo gairdneri*) and zebra fish (*Brachiodanio rerio*). Based on the toxicity values for 1-hexene from five tests, this chemical can be characterized as moderately toxic to aquatic organisms (acute toxicity >1 mg/L and <100 mg/l; EPA, 1992). Rainbow trout demonstrated the greatest sensitivity to this chemical in the five tests reported. The 96-hr LC50 value was 5.6 mg/L. In comparison, the zebra fish, Daphnid and algal data suggest that these organisms are less sensitive. However, it is questionable that the test systems used, other than the rainbow trout, were able to maintain consistent concentrations throughout the duration of the test. Therefore, it is likely that these data do not accurately characterize the acute toxicity of 1-hexene to the organisms. For example, the acute toxicity to algae was reported in the study as a 96-hour EC50 of 1000 mg/L based on cell counts. However, in reviewing the study it was determined that five of the doses used in the study were above the water solubility value for 1-hexene (~ 50 mg/L). As a result, it was determined that the actual 96 hour EC50 was 22 mg/L; the highest nominal concentration used below the water solubility level with 50% of algae affected. Further evidence of 1-hexene aquatic toxicity is provided by calculated data. Calculated endpoint values for a green alga, Daphnid, and a fresh-and saltwater fish suggest that 1-hexene would exhibit a relatively narrow range of toxicity between 1.3 to 3.6 mg/L. This is in general agreement with the measured rainbow trout data.

b. 1-Octene: Toxicity data are available for an alga (*Selanastrum capricornutum*), Daphnid (*Daphnia magna*), and zebra fish (*Brachiodanio rerio*). Measured toxicity studies were conducted using pure octene in the daphnid and fish studies, and a blend mixture containing alpha olefins C_6-C_8, Olefin 68 PQ11 for the algal study. Only 16% of the mixture contained octene. The chemical tested was not completely soluble at all concentrations tested and concentrations were expressed in terms of the amount initially added. Based on the toxicity values for 1-octene from the Daphnid and fish tests, this

chemical can be characterized as moderately toxic to aquatic organisms. Acute values for the two organisms range from 3.2 to 10 mg/L. Although the data used to characterize algal toxicity suggests a lower order of toxicity (96 hour EC50 of 200 mg/L based on cell counts), the study may not have adequately maintained concentrations of test material throughout the duration of the test. The calculated data cover a narrow range from 0.25 to 0.4 mg/L. Although the calculated data suggest that 1-octene may be more toxic to these organisms than the test values actually indicate, there is no reason from the information provided to consider the test data questionable.

c. 1-Decene: Toxicity values for algae, invertebrates, and vertebrates are reported. Measured toxicity studies were conducted using a blend mixture containing alpha olefins C_{10} through $C_{13,}$ Shop Olefin 103. The blend contained 30% of the C_{10}-C_{11} compounds.

Acute measured toxicity tests are reported for an alga (*Selenastrum capricornutum*), Daphnids (*Daphnia magna*), and rainbow trout (*Salmo gairdneri*). The acute toxicity of C_{10} - C_{13} alpha olefins to the alga was determined in a 4-day growth test. The 96 -hr EC50, based on cell counts was calculated to be 22 mg/L. The toxicity of the test material to a Daphnid was determined in a static test. The 24 and 48-hr EC50 values were 720 mg/L and 480 mg/L, respectively. The estimated fish LC50 of >1000 mg/L may not accurately characterize the toxicity of this alpha olefins because the effect concentrations far exceed the water solubility (0.115 mg/L). In addition, the validity of these data is questionable because the test vessels were not sealed and would have lost test material from the test systems through volatilization.

Acute predicted toxicity for 1-decene to an alga was considered highly toxic (predicted value <1 mg/L EPA, 1992). Only algal values could be predicted from the model because of the high log P_{ow} value, a detailed explanation is located in Appendix B.

d. 1-Dodecene: Toxicity values for algae, invertebrates, and vertebrates were the same ones reported above for 1-decene, which used a blend mixture containing alpha olefins C_{10} through C_{13}. Only 11% of the mixture contained 1-dodecene. The chemical tested was not completely soluble at all concentrations tested and concentrations were expressed in terms of the amount initially added.

ECOSAR could not be utilized to predict aquatic toxicity for 1-dodecene because of its high log P_{ow} value (see Appendix B).

e. ***1-Tetradecene***: Toxicity data are available for algae (*Selenastrum capricornutum),* Daphnid (*Daphnia magna*) and fish, rainbow trout (*Salmo gairdneri*). Results of three studies with these organisms showed that test media saturated with the test chemical at a test material loading of 1000 mg/L did not produce toxic effects. The results were: algal 96-hr EL0 = 1000 mg/L, based on biomass; Daphnid 48-hour EL0 = 1000 mg/L; and trout 96-hour LL0 = 1000 mg/L (EL = effect loading; LL= lethal loading; EL/LL0 = no effects or toxicity at the loading referenced). The test procedure used water accommodated fractions (WAFs) of the test material. This type of test procedure evaluates the toxicity of poorly water-soluble materials up to their maximum water solubility limit at the specified test material loading. A WAF is prepared by mixing a test material (organic phase) with a measured volume of aqueous test medium for a period of time sufficient for the test material to reach saturation in the medium, then separating the aqueous phase from the remaining organic phase and evaluating for toxicity. Based on the results from these tests, this chemical can be characterized as not being sufficiently water soluble to cause toxicity to algae or acute toxicity to Daphnids and fish.

The ECOSAR model was unable to predict the acute toxicity of 1-tetradecene because of the chemical's low water solubility. (Please see Appendix B)

B. Chronic Aquatic Toxicity: Chronic toxicity data were not available for the C_6-C_{14} Alpha Olefins. The chronic data presented in this SIAR were calculated using the ECOSAR model (see Appendix B). Table 5B lists the chronic 30-day fish values for selected alpha olefins from 1-hexene to 1-dodecene, as increasing in toxicity from 0.496 to 0.004 mg/L, respectively. ECOSAR was not able to calculate the chronic toxicity of 1-tetradecene due to model limitations of chemicals with higher Kow values.

C. Bioconcentration Factors (estimated): Based on ECOSAR and EPWIWIN model predictions, 1-hexene (81), octene (659), decene (488) and dodecene (313) indicate moderate values while tetradecene's (1586) is considered high. There appears to be a small decrease in BCF potential from octene to dodecene. (EPIWIN, 1999 and Franke et al, 1994)

4.2 Terrestrial Effects:

There were no terrestrial toxicity studies found for the alpha olefins.
Based on level III fugacity modeling, the estimated partitioning of the alpha olefins indicates these chemicals have the potential to partition to the sediment and soil compartments if released to the environment.

Table 5A: Algae Toxicity and Invertebrate and Fish Acute Toxicity of the C6-C14 Alpha Olefins

Species	Measured / Predicted	Duration	Endpoints (mg/L)	Comments
1-Hexene – All experimental values used 1-hexene >96%.				
Algae				
(*Selenastrum capricornutum)*	Measured	96-hr EC0	22	Endpoint was biomass; no attempt to prevent evaporation.
Green Algae	Predicted	24-hr EC50	2.4	
Invertebrate				
(Daphnia magna)	Measured	48-hr EC50	30-60	
(Daphnia magna)	Measured	48-hr EC50	230	Static, test result is above water solubility; no attempt to prevent evaporation
Daphnid	Predicted	24-hr EC50	3.6	
Vertebrates				
Rainbow trout (*Salmo gairdneri)*	Measured	48-96-hr LC50	5.6	Semi-static, minimal headspace to prevent losses through evaporation
Zebra fish (*Brachiodanio rerio*)	Measured	96-hr LC50	25-50	Semi-static, stirred 4 h before adding fish, glass beaker covered with a watch glass; also tested in glass-stoppered flask
Freshwater Fish	Predicted	96-hr LC50	3	
Saltwater Fish	Predicted	96-hr LC50	1.3	
1-Octene– All experimental values utilized octene >99% except for the algal test[1]				
Algae				
(*Selenastrum capricornutum*)	Measured	48-hr EC50	200	Endpoint was biomass; no attempt to prevent evaporation; reported value exceeds water solubility limit
Green Algae	Predicted	96-hr EC50	0.30	
Invertebrate				
(Daphnia magna)	Measured	24 hr EC50	>3.2<10	Static, stirred 4 h before adding test animals, glass beaker covered with a watch glass; also tested in glass-stoppered flask
Daphnia	Predicted	24-hr EC50	= 0.40	
Vertebrates				
Zebra fish (*Brachiodanio rerio*)	Measured	24-96-hr LC50	3.2	Static, stirred 4 h before adding fish, glass-stoppered flask, open and closed, nominal with t-butanol as carrier. Without t-butanol as a carrier, the 48-96 hr LC50= 4.8
Freshwater Fish	Predicted	96-hr LC50	0.32	
Saltwater Fish	Predicted	96-hr LC50	0.25	
1-Decene & 1-Dodecene– Test substance utilized was a blend.[2]				
Algae				
Selenastrum capricornutum	Measured	96 hr EC50	22	Static, vessels not sealed, solution aerated. Concentrations utilized in testing were greater than the water solubility
Green Algae	Predicted	96 hr EC50	0.037	For 1-decene only
Invertebrate				
Daphnia magna	Measured	24 hr EC50	720	Static, vessels not sealed, solution aerated Concentrations utilized in testing were greater than the water solubility
Daphnia magna	Measured	48 hr EC50	480	
Daphnid	Predicted	48 hr EC50	0.048	For 1-decene only
Vertebrates				
Rainbow trout (*Salmo gairdneri)*		96 hr LC50 =	>1000	Semi-static, vessels not sealed, solution aerated Concentrations utilized in testing were greater than the water solubility
	Predicted	96 hr LC50	0.035	For 1-decene only
1-Tetradecene – Test substance was 99% C14; WAFs[3]				
Algae				
Selenastrum capricornutum	Measured	72- 96 hr ELO	1000	Growth; static test
Invertebrates				
Daphnid (*Daphnia magna)*	Measured	24 hr EL0	1000	Immobility; semi-static test
Daphnid (*Daphnia magna)*	Measured	48 hr EL0	1000	Immobility; semi-static test
Vertebrates				
Rainbow trout (*Salmo gairdneri)*		96 hr LL0	1000	Mortality; semi-static test

[1]Olefin 68 PQ11 (C_6 = 48%, C_7= 36% and C_8=16%)
[2]Shop Olefin 103 = C10-C11=30%, C11-C12=31%, C12=11% and C13=21%
[3]WAF = Water Accommodated Fractions test procedure was used due to the low water solubility of the test material.
[4]Prediction is for 1-decene only.
EL0 = effect loading based on the WAF testing procedure; no effect observed at the highest loading indicated
LL0 = lethal loading based on the WAF testing procedure; no mortality observed at the highest loading indicated
All predicted values were obtained using Log K_{ow} values obtained from CLOGP

Table 5B: Predicted Chronic Toxicity to Fish.

Chemical	30-Day Chronic Value (mg/L).
1-Hexene	0.496
1-Octene	0.06
1-Decene	0.008
1-Dodecene	0.004
1-Tetradecene	Model not utilized, please see Appendix B

All predicted values were obtained using Log K_{ow} values obtained from CLOGP

5. Category Discussion:

The five alpha-olefins discussed in this SIAR have been brought together as a category for the purposes of the OECD SIDS Programme. Thus, this discussion will center on whether the proposed test plan- to treat the five chemicals as a category – was satisfactory.

Physiochemical Properties:

Table 1B clearly shows a distinct trend or pattern from the shortest AO (C_6) to the longest AO (C_{14}) for each of the properties listed. Melting point, vapor pressure, and water solubility decreases with increasing chain length whereas, boiling point, log K_{ow}, Henry's Law Constant, and the soil sorption coefficient all increase with increasing chain length. Most of the listed values are measured (melting and boiling points, vapor pressure and some log K_{ow} and water solubility values). However, there is no need to acquire measured log K_{ow} (C_{14})or water solubility values(C_{12} and C_{14}) for the category members for which these data are missing. Due to the knowledge gained from the trend analysis for both parameters, C_{14} would likely have a very high Log K_{ow} and very low water solubility and the C_{12} water solubility would also be quite low.

Environmental Fate and Transport:

A variety of measured and estimated data are presented in Table 3 that characterize the environmental fate and transport of the five category members. Using appropriate input values rather than the defaults, the fugacity Level III distribution model suggests distribution to water will decrease with increasing chain length, distribution to sediment will increase with increasing chain length and distribution to air will be similar for hexene and octene ($\geq$ 15%) and for decene, dodecene and tetradecene ($\leq$ 5%). These results seem reasonable given the physico/chemical properties mentioned above.

Movement of the alpha olefins through soil is affected by both the soil sorption coefficient and volatility, and it is estimated that such movement will be moderate to rapid for hexene, but will decrease with increasing chain length to negligible mobility for tetradecene.

The available data on biodegradation (experiments performed with hexene, decene, dodecene, and tetradecene) suggest that, qualitatively speaking, all are readily biodegradable. From a category perspective there does not appear to be an easily defined increasing or decreasing trend. The same is true for the atmospheric oxidation estimates – all five category members appear equal.

In the final analysis, sufficient information is available on select members of the alpha olefin category for all the major SIDS environmental fate/transport endpoints so that further individual testing is not needed.

Human Health:

Data presented relative to the health toxicity endpoints of the C_6-C_{14} alpha olefins indicate no differences among the five category members for acute toxicity, repeat dose toxicity, genotoxicity, and reproductive/developmental toxicity. Importantly, there are data available on all five category members for acute toxicity and genotoxicity SIDS

endpoints. Repeat dose toxicity data are available for hexene, octene, and tetradecene and reproductive/developmental toxicity data are available for hexene and tetradecene.

The repeat dose toxicity results suggest that octene (NOEL of 50 mg/kg for male rats) appears to be more toxic than either hexene or tetradecene (both showing NOELs of 100 mg/kg for males). The octene data point suggests that any category pattern that might exist (equal toxicity across all members) given the hexene and tetradecene data might not exist for the middle members of the category. However, upon closer review of the octene data, it is seen that the doses used in the repeated dose study were 5, 50 and 500 mg/kg. Since the LOEL was 500 mg/kg, the "true" NOEL is anywhere from 50 to 500 mg/kg. Therefore, given these data, it is believed that all members of the category are likely to have equal general toxicity under repeated dose conditions. Finally, it should be noted that in all cases, male rats were more sensitive than female rats. In the octene and tetradecene repeated dose studies as well as in the hexene combined reproductive/developmental toxicity study, histological lesions were observed in the kidneys of male rats only. In most of the cases, there was documentation of accumulation of hyaline droplets in the proximal convoluted tubules of the kidney, but there was no verification whether the $alpha_{2u}$ – globulin protein was present. Nonetheless, the effect was treatment-related, confined to males, and is consistent with the male-rat specific kidney effect that does not appear to be relevant to humans.

Data are only available for C_6 and C_{14} regarding reproductive and developmental toxicity. As with the repeated dose data the results are relatively the same. Given the results of the general toxicity data it appears that all members would also have equal toxicity values across the category for reproductive and developmental toxicity. Therefore a consistent pattern appears to be established for the alpha olefins and, for the purposes of the OECD SIDS Programme, there is no need to conduct further SIDS-level health tests for repeat dose, reproductive, or developmental toxicity with decene and dodecene.

Ecotoxicity:

The measured aquatic toxicity data (Table 5A) indicate that the C_6 to C_{14} alpha olefins are divided into two subgroups; the lower alpha olefins, C_6 to C_{10}, that exhibit acute effects at levels below their water solubility; and the higher olefins, C_{14} and possibly C_{12}, that do not exhibit acute toxicity because they cannot achieve a concentration in water sufficient to produce acute toxicity.

Qualitative results (placing either the measured or numeric estimate of the acute toxicity value presented in Table 5A into qualitative concern categories per EPA, 1992) of the acute predicted ecotoxicity values (Tables 6) indicate that C_8 through C_{10} are similar for algae, daphnids, and fish and C_6 and C_{14} are in subcategories by themselves. Chronic predicted toxicity values (Table 7) indicate that C_6 through C_{12} are similar in toxicity while C_{14} remains in a category by itself.

TABLE 6: Acute Aquatic Toxicity of Alpha Olefins

Chemical Name	Algae		Daphnids		Fish	
	Measured	**Predicted**	**Measured**	**Predicted**	**Measured**	**Predicted**
1-hexene	Low	Moderate	Moderate	Moderate	Moderate	Moderate
1-octene	Low	High	Moderate	High	Mod-Low	High
1-decene	Moderate	High	Low	High	Low	High
1-dodecene	Moderate	High	Low	*	Low	*
1-tetradecene	Low	*	Low	*	Low	*

*Exceeds to K_{ow} cutoff value.
*unable to predict due to the chemicals low water solubility
High < 1 mg/L, Moderate >1<100 mg/L, Low >100 mg/L (EPA, 1992)

TABLE 7: Chronic Aquatic Toxicity of Alpha Olefins

Chemical Name	**Fish**
1-hexene	Moderate
1-octene	High
1-decene	High
1-dodecene	High
1-tetradecene	*

*unable to predict due to the chemicals low water solubility however, the hazard is assumed to be similar to that of 1-dodecene based on general chemical properties and environmental fate data.
High <0.1, Moderate 0.1 – 10, Low > 10 mg/L (EPA, 1992)

6. Conclusions and Recommendations

Conclusions:

Since C_6-C_{14} alpha-olefins are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals, human exposure is expected to be minimal. Distribution modeling suggests that any environmental releases would result in the majority (>50%) of lower chain length alpha olefins (hexene and octene) partitioning to water and the remaining, higher chain length alpha olefins (decene, dodecene, and tetradecene) partitioning to soil/sediment.

The higher the carbon chain length is, the greater the tendency for the chemicals to bind to particulate matter. With increasing Log K_{ow}, there is a decrease in persistence in the water. However, with increase in the log Kow value, there is an increase in persistence in the soil/sediment compartments (see Table 3). The biodegradation process of the alpha olefins varies from days to weeks under aerobic conditions. Volatilization is predicted to occur rapidly because of the high Henry's Law constant and vapor pressure. Based on calculated octanol/water partition coefficients and bioconcentration factors, tetradecene is the only category member that may have the potential to bioaccumulate.

The C_6-C_{14} alpha olefins indicate a low toxicity concern following acute oral, dermal, and inhalation exposures. These compounds are slightly irritating to the skin (pure materials only) and eyes (pure materials or mixtures) of rabbits. From a category perspective, it is interesting that the alpha-olefin blends appear to be skin irritants, but not eye irritants. There does not seem to be a noticeable difference in irritation by carbon chain length. They do not cause sensitization in guinea pigs. Repeated oral dose studies show that these alpha olefins target the male rat kidney; and 1-tetradecene produces slight increases in hepatocytic cytoplasmic vacuolation and liver weights at high doses. The kidney effects are likely related to $alpha_{2u}$ globulin caused hydrocarbon nephropathy, which is not considered relevant to human health. Based on screening level studies it appears that the C_6-C_{14} alpha olefins do not indicate signs of neurotoxicity; reproduction or fetal development effects; or genotoxicity. Aspiration into the lung after oral ingestion is a potential hazard; however, ingestion is not an expected route of human exposure. Thus, adverse effects from occupational or non-occupational exposure to C_6-C_{14} alpha olefins is expected to be minimal.

If alpha olefins enter the water compartment, measured acute aquatic toxicity data indicate a low to moderate concern depending on the alpha olefin and the species of concern. Table 6 indicates that 1-hexene is moderately toxic to invertebrates and fish and low for algae; while the reverse is true for decene and dodecene. Toxicity values for 1-octene are moderate for algae, low for invertebrates and moderate-low for fish. 1-Decene and 1-dodecene toxicity values are considered to be moderately toxic to algae. From a category perspective, a trend appears to be present for the alpha olefins for daphnids and fish (decreasing toxicity with increasing chain length). This does not appear to be true for algae. The ECOSAR predictions for acute toxicity were in general agreement with the measured values (Table 6), although they did overestimate toxicity in many cases.

1-Hexene and 1-octene have demonstrated moderate toxicity to aquatic organisms under closed test systems. Under open conditions, which are considered to be more relevant to actual environmental exposures, the C_6-C_{14} alpha olefins have indicated through testing values to be a low concern for toxicity. Predicted acute and chronic data indicate that the alpha olefins toxicity

increases with increasing chain length. However, the higher end chains are not likely to be bioavailable to aquatic organisms because of the high vapor pressure and low water solubility.

Predicted chronic aquatic toxicity data indicate that 1-hexene may be moderately toxic and all the other alpha olefins (except 1-tetradecene) may be highly toxic to fish.

Recommendations:

The category of alpha olefins should be considered a candidate for further work in the OECD SIDS Program. Further work is recommended in the environmental area. There are no measured data available for chronic toxicity to aquatic organisms; however, computer modeling suggests that 1-octene, 1-decene and 1-dodecene may be highly toxic (chronic value<0.1 mg/L) under chronic exposure conditions. Therefore it is recommended that further data be collected from member countries regarding actual release data from manufacturing and processing facilities to the water compartment at local and national levels. In the event that releases to the water compartment are occurring at levels anticipated to pose a hazard to the aquatic environment, then consideration should be given to determining if chronic aquatic toxicity testing (including sediment-dwelling organisms) would be appropriate.

The exposure potential to workers presented by these chemicals is low. The data on potential human health effects indicate low hazard to exposed populations.

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APPENDIX A

Environmental exposure for 1-decene

Assessment of releases of 1-decene to the environment is based on modeling, as no measured data is available. Emissions have been estimated from production and processing of 1-decene.

Releases from production

There is no information in the SIAR for alpha olefins on the volume of releases from the production of 1-decene. Therefore estimates from the EU Technical Guidance Document for risk assessment of new and existing substances (TGD) will be used. There is no accurate data available on the total production volume of 1-decene in Europe or in USA. 30 000 tons is taken as the capacity of presumably typical manufacturing site. If the production operates 300 days per year then the daily production rate is 100 tons. Based on the release tables in the EU Technical Guidance Document (using industrial category: chemicals industry, chemicals used in synthesis) emission factors are:

to air: 0.1 %
to water: 0.3 %
to soil: 0.01 %.

These give 100 kg/day released to air, 300 kg/day to water and 10 kg/day to soil.

Releases from processing

1-Decene is used as an intermediate in the production of synthetic lubricants, synthetic fatty acids, OXO alcohol etc. as mentioned in the SIAR for alpha olefins (see Table 2). Based on the information received from the European processors of 1-decene, 50 000 tons is taken as the capacity of a typical processing plant. If the processing operates 300 days per year then the daily processing rate is 166.7 tons. As no release estimates have been presented in the SIAR for alpha olefins, estimates from the EU Technical Guidance Document have been used. Emission factors are (using industrial category: chemicals industry, chemicals used in synthesis) :

to air: 0.01 %
to water: 0.7 %
to soil: 0.01 %.

These give 17 kg/day released to air, 1167 kg/day to water and 17 kg/day to soil.

Predicted Environmental Concentrations (aquatic)

Production

It is assumed that the aqueous release of 300 kg/day goes to a sewage treatment plant (STP) with a capacity of 2000 m^3 /day, giving a concentration in the inflow of 150 mg/l. 1-decene can be regarded as readily biodegradable, but failing the 10-day window. The tables in the Technical Guidance on removal percentages based on physico-chemical properties (1-decene: log Kow = 5.7 and log H = 5.6) give a distribution of 62.6 % to sludge , 30 % to air, 4 % degraded and 3.45 % to water. This gives a concentration in the effluent of 5.17 mg/l. Assuming a default dilution factor of 10 gives the concentration in the receiving waters as 0.517 mg/l = **517 µg/l**.

Processing

It is assumed that the aqueous release of 1167 kg/day goes to a sewage treatment plant (STP) with a capacity of 2000 m^3 /day, giving a concentration in the inflow of 583.5 mg/l. The tables in the Technical Guidance on removal percentages based on physico-chemical properties (1-decene: log

Kow = 5.7 and log H = 5.6) give a distribution of 62.6 % to sludge , 30 % to air, 4 % degraded and 3.45 % to water. This gives a concentration in the effluent of 20.1 mg/l. Assuming a default dilution factor of 10 gives the concentration in the receiving waters as 2.01 mg/l = **2010 µg/l.**

Predicted Environmental Concentrations (atmosphere)

As no data on effects to plants or some other organism which are exposed via atmosphere are available, no PNECs or PECs have been calculated.

Predicted Environmental Concentrations (soil)

In the calculation of 1-decene concentration in soil exposure from the application of sewage sludge in agriculture and dry and wet deposition will be considered. In these calculations sludge application rate of 0.5 kgdw/m^2/year is assumed. The concentration in soil will be high just after the sludge application and will reduce in time due to removal processes (degradation, volatilization and leaching). Therefore the concentration is averaged over 30 days after application of sludge. The contribution to the overall impact from wet and dry deposition is based on the emission calculation of a point source within 1000 m from that source. Atmospheric deposition is assumed to be a continuous flux throughout the year. Calculations have been carried out with the EUSES-model.

Predicted concentration of 1-decene in agricultural soil will be **43.2 mg/kg** (wet weight) from production and **168 mg/kg** (wet weight) from processing.

APPENDIX B

Documentation for Models used in the Alpha Olefins SIAR: EPIWIN Suite, ECOSAR and EQC Fugacity Model

EPIWIN Suite

The EPI Suite is a combination package that includes the EPIWIN Program, the SMILECAS Database, and ten separate estimation programs. The EPIWIN Program (Estimations Programs Interface) is an interface that transfers a single SMILES notation to ten separate structure estimation programs that require SMILES notations. The ten programs (AOPWIN, BCFWIN, BIOWIN, ECOSAR, HENRYWIN, HYDROWIN, KOWWIN, MPBPWIN, PCKOCWIN, and WSKOWWIN) are all standalone programs; they do *not* require EPIWIN to run. Although these ten programs are not actually part of EPIWIN itself, EPIWIN was designed specifically to execute them and capture their output. The EPIWIN interface program is a convenience for users because it automatically executes each program in succession without user interaction. In addition, the interface program executes the WVOLWIN (Volatilization Rate from Water) and STPWIN (Sewage Treatment Plant Fugacity Model) programs by transferring the Molecular Weight, the Henry's Law Constant, log octanol-water partition coefficient and various volatilization parameters to WVOLWIN and STPWIN. Any of the estimation programs (with the exception of STPWRN and WVOLWIN) can be run by themselves. The STPWIN program is a version of the Toronto Model originally developed by Donald Mackay at the University of Toronto and estimates removability by volatilization, adsorption to sludge and biodegradation. The WVOLWIN program is based upon the methodology outlined in Chapter 15 of W.J. Lyman's book "Handbook of Chemical Property Estimation Methods" (Lyman et al., 1990). Mackay's Level III fugacity model has been added to the EPI Suite.

AOPWIN

The Atmospheric Oxidation Program (AOPWIN) estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. It also estimates the rate constant for the gas-phase reaction between ozone and olefinic/acetylenic compounds. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals and ozone.

The estimation methods used by the Atmospheric Oxidation Program are based upon the structure-activity relationship (SAR) methods developed by Dr. Roger Atkinson and co-workers (Atkinson, 1987, 1988; Atkinson and Carter, 1984; Kwok and Atkinson, 1995). A journal article describing the AOP Program has been published (Meylan and Howard, 1993). In addition, some new fragment and reaction values have been derived from new experimental data.

BCFWIN

The Bioconcentration Factor Program (BCFWIN) is a recent addition to the EPI Suite of estimation programs. The methodology was developed under contract with the U.S. EPA from a training set of 694 compounds with measured BCF values in fish (Meylan et al., 1997, 1998). BCF is estimated from the octanol-water partition coefficient (log P) and a series of structural correction factors. BCFWIN can estimate BCF for ionic compounds.

BIOWIN

The Biodegradation Probability Program (BIOWIN) estimates the probability for the rapid aerobic biodegradation of an organic chemical in the presence of mixed populations of environmental microorganisms. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses. A discussion of the methodology used to derived the linear and non-linear fragment constants is presented in a journal article by Howard et al., 1992. Experimental biodegradation data for the multiple linear and non-linear regressions were obtained from Syracuse Research Corporation's (SRC) data base of evaluated biodegradation data (Howard et. al., 1987).

BIOWIN version 3 was updated to include expert judgement estimates for the time required to achieve primary and ultimate biodegradation. Boethling et al., 1994 gives a complete description of the methodology.

ECOSAR

The Ecological Structural Activity Relationship (ECOSAR) Class Program is a computerized version of the ECOSAR analysis procedures as currently practiced by the EPA Office of Pollution Prevention and Toxics (OPPT). It has been developed within the regulatory constraints of the Toxic Substances Control Act (TSCA). It is a pragmatic approach to SAR as opposed to a theoretical approach.

The structure-activity relationships (SARs) presented in this program are used to predict the aquatic toxicity of chemicals based upon their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. Most SAR calculations in the ECOSAR Class Program are based upon the octanol/water partition coefficient (Kow). Various surfactant SAR calculations are based upon the average length of carbon chains or the number of ethoxylate units.

EPA policy, set out in the Federal Register (December 1, 1993, 58 FR 63506) is to use this model where no or insufficient actual aquatic toxicity data exist upon which to base a decision.

The ECOSAR program predicts the acute toxicity of a chemical to fish (both fresh and saltwater), water fleas (daphnid), and green algae.
Some limitations apply when using the model for the alpha olefins. Because these chemicals are categorized as neutral organic, the ability to predict the acute toxicity is influenced by the log K_{ow} (octanol/water partition coefficient) of the chemicals. For fish (both fresh and saltwater) and daphnid, the cutoff for predicting acute toxicity is a log K_{ow} of five. For green algae, it is 6.4. The cutoff point for chronic toxicity is 8.0.

Since there are no measured data available in the literature for chronic aquatic toxicity or persistency for the aforementioned chemicals, ECOSAR/EPIWIN was used to predict these endpoints. The values of the parameters used in the models are presented below.

Values used in ECOSAR for Predicting the Toxicity of Alpha Olefins

Chemical	Log K_{ow}	M.W.	M. P. (EC)	B. P. (EC)	V. P. (mm Hg)	H.L.C. (atm m^3/mol)	K_{oc}	W. S (mg/L)
1-hexene	3.39	84.16	-139.7	63.4	184	0.412	149	50
1-octene	4.57	112.22	-102	121	17.4	0.627	507	4.1
1-decene	5.70	140.27	-66.3	170.5	1.67	2.68	1724	0.115
1-dodecene	6.1	168.33	-35.2	213.8	0.159	4.25	5864	0.113
1-tetradecene	7.08	196.38	-13	251	1.5×10^{-2}	8.48	19950	$4X10^{-4}$

FUGACITY LEVEL III

Level III fugacity model of Mackay (Mackay D., Paterson S., and Shiu W.Y., 1992) determines the persistence of a chemical substance in the environment. The Level III fugacity model is multi-media model that uses a chemical's physical/chemical properties and degradation rates in air, water, soil and sediment. The Level III fugacity model has been validated in numerous studies Kuhne R. et al. 1997; Matoba Y. et al. DATE; Suzuki N. et al. 1998). The fugacity model requires a series of physical/chemical properties and environmental parameters as input. These are provided by SRC's EPIWIN suite of structure-based estimation programs [http://esc.syrres.com/~esc/estsoft.htm]. Physical properties are used directly by the fugacity model to determine the transport between environmental compartments. These properties, and citations to the methodology used for each property, are Henry's Law constant (Meylan, W.M. and Howard, P.H., 1991); vapor pressure (Lyman, W.J., Reehl, W.F.and Rosenblatt, D.H., 1990), melting point (Stein, S.E. and Brown, R.L., 1994; Reid, R.C., Prausnitz, J.M., and Poling, B.E., 1987); water solubility (Meylan, W.M. and Howard, P.H. 1996); octanol/water partition coefficient (Meylan, W.M. and Howard, P.H., 1996); and molecular weight.

The fugacity model also requires a half-life input for air, water, soil, and sediment. Atmospheric half-lives are calculated by SRC's electronic version of the fugacity model using gas-phase hydroxyl radical and ozone reaction rate (Meylan, W.M. and Howard. P.H. 1993) and the average atmospheric concentration of these oxidants (Prinn, R.., et al, 1992); Atkinson, R. and Carter, 1984). Half-lives for water, soil, and sediment are determined using the ultimate biodegradation expert survey module of the BIOWIN estimation program (Boethling, R.S., et al, 1994).

EQC Model vs EPIWIN fugacity Model: The EQC model available from Trent University (www.trentu.ca/envmodel) was utilized to generate the output for the Level I and III fugacity models presented in this SIAR. Because Level I and Level III give different results and inputs can be manipulated in running level III models, the following model runs were made.

A. Level I = default emissions of (1,000 kg/hr)
B. Level III = EPIWIN default emissions of (1,000 kg/hr to air, water and soil compartments)
C. Level III = EQC model inputs based on Exxon Estimates of release (10 kg/hr to air, 1 kg/hr to water, 0 kg/hr to soil)

Results were as follows:

	Environmental Compartment	A. Level I **(%)**	**B. Level III using default emission values in EPIWIN (%)**	**C. Level III using Exxon estimated releases, EQC model (%)**
HEXENE	**Air**	100	8.5	21
	Water	<1	83.1	77
	Soil	<1	8.02	<1
	Sediment	<1	0.385	2
OCTENE				
	Air	99.7	5.52	15
	Water	<1	56.3	61
	Soil	<1	34	<1
	Sediment	<1	4.08	23
DECENE				
	Air	99.2	2.4	5
	Water	<1	30.4	19
	Soil	<1	45.1	<1
	Sediment	<1	22	76
DODECENE				
	Air	84.9	1.24	3
	Water	<1	19.6	12
	Soil	14.7	53.4	<1
	Sediment	<1	25.8	85
TETRADECENE				
	Air	94.9	1	5
	Water	<1	14	6
	Soil	5	50	<1
	Sediment	<1	35	89

HENRYWIN

The Henry's Law Constant program (HENRYWIN) estimates the Henry's Law Constant (HLC) of organic compounds at 25 deg C using the methodology originally described by J. Hine and P.K. Mookedee (1975). The original methodology was updated and expanded by Syracuse Research Corporation (Meylan and Howard, 1991) and presented in the software program HENRY (version 1). A subsequent update (HENRYWIIN version 2) included additional fragment and correction factors. HENRYWIN version 3 extends the methodology to allow estimation of Henry's law constant over a temperature range (0 to 50 deg C). In addition, version 3 includes an experimental Henry's law constant database of 1150 compounds.

HYDROWIN

The HYDROWIN program estimates aqueous hydrolysis rate constants at 25 deg C for selected chemical classes. The selected chemical classes in the current version include esters, carbamates, epoxides, halomethanes and selected alkyl halides. Rate constant estimates are based solely upon the chemical structure of a compound and are calculated from regression equations derived from experimental hydrolysis data (Mill et al., 1987).

HYDROWIN predicts either acid-catalyzed or base-catalyzed rate constants. It does not estimate neutral hydrolysis rate constants. The estimated acid- or base-catalyzed rate constants are used to calculate hydrolysis half-lives at selected pHs.

KOWWIN

The Log Octanol-Water Partition Coefficient Program (KOWWIN) estimates the logarithmic octanol-water partition coefficient (log P) of organic compounds. A journal article by Meylan and Howard (1995) describes the program methodology (atom-fragment contribution method).

KOWWIN includes a database of more than 12,570 reliable, experimental log P values for different compounds. The database is supplied in two formats: (1) a format that the KOWWIN searches during program execution to match input structures with the database to inform the user that an experimental value exists, and (2) a text version that includes the experimental log P value, the value estimated by KOWWIN and the value estimated by the ClogP Program (BioByte Corporation).

MPBPWIN

The MPBPWIN Program estimates the boiling point, melting point, and vapor pressure of organic compounds. The estimation methodology for boiling point is an SRC adaptation of the Stein and Brown (1994) method. Melting point is estimated by two different methods; the first is an SRC adaptation of the Joback Group Contribution Method (Joback, 1982; Reid et al., 1987), and the second is a Gold and Ogle method (Lyman, 1985) which simply uses the following formula: Tm = 0.5839 Tb where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Although melting point estimation can be inaccurate, we have found that averaging the results of these two methods can yield reasonable estimates for many structures. Vapor pressure is estimated by three methods; all three methods use the normal boiling point. The first is the Antoine method (Chapter 14 of Lyman et al., 1990). The second is the modified Grain method and the third is the Mackay method (see Lyman, 1985). In general, the modified Grain method is preferred for solids, while a combination of the Antoine and Grain method is preferred for liquids. The MPBPWIN determines a best estimation result for all three physical properties.

PCKOCWIN

The PCKOCWIN program estimates the soil sorption coefficient (Koc) of organic compounds. Koc is defined as "the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium" (Lyman, 1990). Koc provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems. PCKOCWIN uses the first-order molecular connectivity index and a series of group contribution factors (derived by Syracuse Research Corp.) to predict Koc. The group contribution method outperforms traditional estimation methods based on octanol/water partition coefficients and water solubility. A discussion of the group contribution method is available (Meylan et al., 1992).

WSKOWWIN

The WSKOWWIN program estimates the water solubility of an organic compound using the compound's log octanol-water partition coefficient (log P) in combination with a series of simple structural correction factors, the molecular weight, and the melting point (the melting point is not required, but can increase accuracy). A description of the estimation methodology is available (Meylan and Howard, 1994a, b. Meylan et al, 1996).

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1-HEXENE (CAS N°: 592-41-6)

FULL SIDS SUMMARY

CAS No.: 592-41-6		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point	N/A	N/A	-139.8 °C
2.2	Boiling Point	N/A	N/A	63.3 °C (at 101 kPa)
2.3	Density	N/A	N/A	0.6731 g/ml @ 20°C
2.4	Vapour Pressure	N/A	N/A	140 mm at 20°C = to 186.5 hPa
2.5	Partition Coeff.(Log Pow)	N/A	N/A	3.39 at 20C (measured)
2.6A	Water Solubility	N/A	N/A	50 mg/l at 20°C
2.6 B	pH/pKa	N/A	N/A	N/A
2.12	Oxidation: Reduction Potential	--	--	-- mV
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation	N/A	Calculated	In air $T_{1/2}$ = 4.2 (hydroxy radical) In air $T_{1/2}$ = 23 hrs (ozone)
3.1.2	Volatilization from water	--	Estimated	$T_{1/2}$ = 0.9 hours (river) $T_{1/2}$ = 3.6 days (lake)
3.1.3	Soil Adsorption		Estimated (C_6)	K_{oc} = 149
3.2	Monitoring Data	N/D	N/D	N/D
3.3	Transport and Distribution		Calculated (Mackay Fugacity Level III)	In Air 21% In Water 77% In Soil <1% In Sediment 2%
			Level 1	In Air 100%
3.5	Biodegradation		(local exposure)	67-98% in 28 days; Readily biodegradable (Japan, MITI)
			closed bottle Sturm Test	22% in 28 days - not readily biodegradable 1-3% in 28 days - not readily biodegradable
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Salmo gairdneri	Static	EL0 (96 hr)= 22 mg/L (nominal)
		Oncorhynchus mykiss	Semi-static	LC_{50} (24 hr) = 9.7 mg/L, LC_{50} (48 hr) = 5.6 mg/L, LC_{50} (72 hr) = 5.6 mg/L, LC_{50} (96 hr) = 5.6 mg/L
		Brachiodanio rerio	Semi-static	LC_{50} (96 hr) = 25 mg/L (closed container) LC_{50} (96 hr) = 50 mg/L (open container)
4.2	Acute Toxicity to Aquatic Invertebrates	Daphnia magna	Static	EC_{50} (48 hr) = 230 mg/l (nominal)
			Static	LC_{50} (48 hr) = 30 mg/l (closed container) LC_{50} (48 hr) = 60 mg/l (open container)
4.3	Toxicity to Aquatic Plants	Algae	4-day Growth experiment	EC_{50} (96 hr) = >22 mg/l (nominal)

CAS No.: 592-41-6		SPECIES	PROTOCOL	RESULTS
4.4	Toxicity to Bacteria	Mixed Marine bacteria	Acute static bioassay	Log LC_{50} = 0.46 (calculated)
		Pseudomonas fluorescens	Microbial Inhibition	Max inhibition was 24% at 1000 mg/l
4.5	Chronic Toxicity to Aquatic Organisms	Daphnia	Predicted using ECOSAR	LC_{50} (48 hr) = 3.633 ppm (predicted) EC_{50} (16-day) = 0.342 ppm (predicted)
		Green Algae		EC_{50} (96 hr) = 2.460 ppm (predicted) ChV (96 hr) = 0.549 ppm (predicted)
		Fish		LC_{50} (96 hr) = 3.080 ppm (predicted) LC_{50} (14 day) = 6.957 ppm (predicted) ChV (30 day) = 0.496 ppm (predicted)
4.6.1	Toxicity to Soil Dwelling Organisms	N/D	N/D	N/D
4.6.2	Toxicity to Terrestrial Plants	N/D	N/D	N/D
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds)	N/D	N/D	N/D
	TOXICOLOGY			
5.1.1	Acute Oral Toxicity	Rat Rat	OECD 401 --	LD_{50} >5600 mg/Kg LD_{50} >10,000 mg/Kg
5.1.2	Acute Inhalation Toxicity	Rat	--	LC_{50} 32,000 ppm
5.1.3	Acute Dermal Toxicity	Rabbit	OECD 402 [except that four males and females were listed]	LD_{50} >2000 mg/Kg
		Rabbit	--	LD_{50} >10,000 mg/Kg
5.2	Dermal Irritation			
5.2.1.	Skin Irritation	Rabbit	OECD 404 [except that exposure was 24 hrs and skin was evaluated only at 24 and 72 hrs.]	Draize = 0.975/8
		Rabbit	---	Draize = 1.0, classified as non-irritating by US OSHA and EU criteria
5.2.2	Eye Irritation	Rabbit	OECD 405 [3 male and female unwashed, 3 male washed]	Max Draize (1 hr) = 8/110 Avg Draize (1 hr) = 5.0/110 (unwashed) Avg Draize (1 hr) = 5.3/110 (washed) Classified as “mildly irritating”
		Rabbit	-----	Draize = 1.7/110; no corneal opacity or iritis
5.3	Skin Sensitization	Guinea Pig	OECD 406 - Buehler	Negative
5.4	Repeated Dose Toxicity	Rat	OECD 413	NOEL = 1000 ppm (inhalation)
		Rat	OECD 407	NOEL = 101 mg/kg (males, gavage) (male rat nephropathy) NOEL >1000 mg/kg (females, gavage)

CAS No.: 592-41-6		SPECIES	PROTOCOL	RESULTS
5.5	Genetic Toxicity In Vitro			
A	Bacterial Test (Gene mutation)	S. typhimurium TA98, TA100, TA1535, TA1537, TA1538	OECD 471 w/out repeat assay	Negative – with and w/out metabolic activation)
		S. typhimurium TA98, TA100, TA1535, TA1537, TA1538	OECD 471 w/out repeat assay	Negative – with and w/out activation
B	Non-Bacterial Test:			
	Chromosomal aberrations	Chinese Hamster Ovary	OECD 473 (duplicative assay but not with duplicate cultures)	Negative - (With and w/out metabolic activation)
		Human lymphocytes	Metaphase chromosome analysis	Negative with or without metabolic activation
	DNA damage/repair	Rat hepatocyte UDS	OECD 482	Negative at 0.5 and 2.0 mg/mL ; no evaluation at 3.5 to 5.0 mg/mL due to toxicity.
	Genetic mutation	Mouse Lymphoma; L51784	Mammalian cell Gene mutation	Negative - with and w/out activation
	Neoplastic transformation	BALB/3T3 cells	--	Negative
5.6	Genetic Toxicity In Vivo Bone marrow micronucleus	Mouse	OECD 474 (inhalation)	Negative
5.8	Toxicity to Reproduction/ Developmental	Rat Rat	OECD 413 OECD 421	NOEL = 1000 ppm (from repeated dose study, see Section 5.4) NOEL = <100 mg/Kg (General toxicity male rat nephropathy) NOEL = >1000 mg/Kg (Reproductive Toxicity, parental, adult female) NOEL = >1000 mg/kg (Reproductive Toxicity, F1generation) NOEL = >1000 mg/Kg (Pregnancy/litter) NOEL = >1000 mg/kg (Foetal data)
5.9	Developmental Toxicity/ Teratogenicity	Rat	OECD 421	See Section 5.8 for combined reproduction/developmental study.

CAS No.: 592-41-6		SPECIES	PROTOCOL	RESULTS
5.10	Specific toxicity: Toxicodynamics/Toxico-kinetics	In vitro System Rat	-- --	Autocatalytic ("suicidal") destruction of cytochrome P-450 and heme in hepatic microsomes from phenobarbital pre-treated rats. Shown to be a substrate for cytochrome P-450 by its binding spectrum to the cytochrome. Conc. Of 1-alkenes in blood tissues increases with an increase in C atoms. In contrast, levels of hemoglobin and DNA adducts decreased with increasing # of C atoms. It is highly unlikely that the higher homologs including 1-hexene will be genotoxic under these conditions.
5.11	Experience with Human Exposure	Human		Narcosis with CNS effects, mucous membrane irritation, vertigo, vomiting and cyanosis when inhaled at a concentration of 0.1%. Prolonged/repeated exposure may cause dry/cracked skin. Recovery expected when removed from exposure area.

N/A = not applicable N/D = not determined

Other information: 1-hexene was a mild eye and skin irritant, but was not a skin sensitizer in guinea pigs [OECD 406 Buehler method]. 1-hexene is classified as a non-irritant by US OSHA and EU criteria.

SIDS DOSSIER
1-HEXENE (CAS No:592-41-6)

SIDS PROFILE

1.1	CAS NO.	592-41-6
1.2	CHEMICAL NAME	1-HEXENE
1.3	STRUCTURAL FORMULA	CH_2 =CH-$(CH_2)_3$-CH_3
2.0	OTHER CHEMICAL IDENTITIY INFORMATION	C6 Alpha Olefin, NEODENE® 6, Gulftene® 6, NERATEN® 6
3.0	SOURCES AND LEVELS OF EXPOSURE*	Manufactured in closed systems; Shell internal standard 100 ppm; Phillips detected 8 hr TLV-TWA of 0.12 ppm; contained at very low levels in refined petroleum products such as gasoline; minor solvent use
3.1	PRODUCTION RANGE	1994 USA annual production - 77,000,000lbs [non-confidential business information]
3.2	CATEGORIES AND TYPE OF USE	Industrial intermediates - comonomer in polyethylene, oxo alcohol intermediate, synthetic fatty acid intermediate
4.0	ISSUES FOR DISCUSSION	Testing completed since the previous dossier indicates 1-hexene does not cause reproductive or developmental toxicity in rats at oral doses as high as 1000 mg/kg/day in an OECD guideline study. The only lesion reported was “hydrocarbon nephropathy ”only in male rats, an effect not considered relevant to human health.

* Data taken from “Information Review [C6-C12] Alkenes, IR-427”. Prepared by CRCS, Inc for EPA, April 30th, 1985.

SIDS SUMMARY

CAS NO: 592-41-6 1-hexene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
PHYSICAL-CHEMICAL								
2.1	Melting Point	Y	N	N	N	N	Y	N
2.2	Boiling Point	Y	N	N	N	N	Y	N
2.3	Vapour Pressure	Y	N	N	N	N	Y	N
2.4	Partition Coefficient	Y	N	N	Y	N	Y	N
2.5	Water Solubility	Y	N	N	N	N	Y	N
OTHER STUDIES RECEVED								
2.6	Flash Point	Y	N	N	N	N	Y	N
2.7	Flammability	Y	N	N	N	N	Y	N
2.9	Density	Y	N	N	N	N	Y	N
ENVIRONMENTAL FATE/ BIODEGRADATION								
3.5	Aerobic Biodegradability	Y	Y	N	Y	N		
3.5	Abiotic Degradability	N						
3.1.2	Hydrolysis	Y	N	N	N	Y	Y	N
3.1.1	Photodegradability	Y	N	N	N	N	Y	N
3.3	Env. Fate/Distribution	Y	N	N	N	Y	Y	N
	Env. Concentration	N						
OTHER STUDIES RECEIVED ECOTOXICOLOGY								
4.1	Acute Toxicity Fish	Y	Y	N	Y	N	Y	N
4.2	Acute Toxicity Daphnia	Y	Y	N	Y	N	Y	N
4.3	Toxicity to Algae	Y	Y	N	N	N	Y	N
4.4	Toxicity to Bacteria	Y	Y	N	N	N	Y	N
4.5.2	Chronic Toxicity to							
	- Daphnia	Y	N	N	N	Y	Y	N
	- Algae	Y	N	N	N	Y	Y	N
	- Fish	Y	N	N	N	Y	Y	N
4.6.1	- Terrest. Organisms	N						
4.6.2	- Terrest. Plants	N						
4.6.3	- Avians	N						
4.6.4	Avian Reproduction	N						
OTHER STUDIES RECEIVED TOXICOLOGY								
5.1.1	Acute Oral	Y	Y	N	N	N	Y	N
5.1.2	Acute Inhalation	Y	N	N	N	N	Y	N
5.1.3	Acute Dermal	Y	Y	N	N	N	Y	N
5.2.1	Corrosivity, Irritation	Y	Y	N	N	N	Y	N
5.2.2	Eye Irritation	Y	Y	N	N	N	Y	N
5.3	Skin Sensitization	Y	Y	N	N	N	Y	N
5.4	Repeated Dose	Y	Y	N	Y	N	Y	N

CAS NO: 592-41-6 1-hexene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
5.5	Genetic Toxicity							
	- Gene Mutation	Y	Y	N	Y	N	Y	N
	- Chromosomal Aberrations	Y	Y	N	Y	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.12	Metabolism	Y	N	N	N	N	Y	N
OTHER STUDIES RECEIVED								

Summary of Responses to the OECD Request for Available Data on HPV Chemicals

REVISED: October 1999

1. General Information

1.01 Substance Information

A. CAS number: 592-41-6

B. Name(IUPAC): 1-hexene

C. Name(OECD):

D. CAS Descriptor: N/A

E. EINECS-Number

F. Molecular formula: C_6H_{12}

G. Structural formula: CH_2 =CH-$(CH_2)_3$-CH_3

H. Substance Group (if possible, only for petroleum products)

I. Substance Remark:

J. Molecular Weight: 84.16

1.02 OECD Information

A. Sponsor Country: United States

B. Lead Organisation: United States Environmental Protection Agency

Mr. Oscar Hernandez, Director RAD
EPA/OPPTS/RAD (7403)
401 M Street, SW
Washington, D.C. 20460
Telephone: (202) 260-1832
Fax: (202) 260-1216

C. Name of Responder:

American Chemistry Council (Higher Olefins Panel)
1300 Wilson Blvd.
Arlington, Virginia 22209, USA

Panel Manager: Doug Anderson
Telephone: (703) 741-5616
Fax: (703) 741-6091

1.1 General Substance Information

A. Type of Substance: Organic

B. Physical State: Liquid (at 20C and 1.013 hPa)

C. Purity of industrial product: Varies, but usually >98%

1.2 Synonyms: hexene-n-1; Butylethylene; Hex-1-ene; Hexylene

1.3 Impurities: Identity of major impurities: Can include 2-Ethyl-1-Butene, Hexane

1.4 Additives: Essential additives (stabilizing agents, inhibitors, other additives), if applicable: None

1.5 Quantity: Production levels expressed as tonnes per annum
U.S.A. 150,000 - 200,000 tonnes (60 million - 150 million pounds)
Reference: b) CRCS, Inc (1985) (1977 TSCA Inventory)

1.6 Labeling and Classification:

International Transport Classification

UN Number	2370
Class	3.1
Packaging group	2
Hazard identity no.	
Proper shipping name	1-hexene
CEFIC-Tremcard no.	
ADR and RID (road, railway)	
Class	3.3b
Symbol	Flammable liquid
Proper shipping name	1-hexene, 3.3b, ADR
IATA/ICAO (air)	
Class	
Packing group	2
Symbol	Flammable liquid
Proper shipping name	1-hexene
IMO/IMDG (sea)	
Class	3.1
Page	3034-5
EMS-No	
MFAG-No	
Packing group	2
Symbol	Flammable liquid 3

EEC-labeling (Shell International recommendation).
Class F - Highly Flammable.
R-phrases - none.
S-phrases - S9, S16, S29, S33

EEC-labeling (Spolana recommendation)
R-phrases -R11-36/37/38-65
S-phrases -S16-24/25-26-46-62

1.7 Use Pattern: Information concerning uses (including categories and types of uses expressed in percentage terms)

Types of uses are divided into three: industrial use (open system and closed system), public use and export

Industrial uses: (Intermediate in the manufacture of : oxo alcohols, alkyl dimethyl amines, surfactants, plastics, $C_5 - C_9$ synthetic fatty acids, lube oil additives, linear mercpatans, alkenylsuccinic anhydrides, epoxides and leather treating compounds.

(In closed systems) Manufacture of copolymers, oxo alcohol intermediates, synthetic fatty acid intermediates.

Public use: Negligible

1.8 Occupational Exposure Limit Value: 100 ppm 8-hr TWA (Shell, 1984)

1.9 Sources of Exposure:

Processes

Petroleum process streams, such as light cycle gasoline contains 1-hexene.

No data are available for workplace concentration. Exposures are expected to be low due to handling in closed systems.

Reference: b) CRCS, Inc. (1985)

Limited to contact with low concentrations of the compounds in ambient air and finished petroleum products. Emissions from manufacturing are expected to be small. On-site waste treatment processes degrade the compounds to the extent that they are not detectable in effluent discharges. Olefins may be released in small quantities by leaks in process equipment used during production of the compounds. They are expected to be released in aqueous effluents and atmospheric emissions from manufacturing and use operations and from fuel processing and combustion. (CRCS, 1985).

1.10 Additional Remarks: Options for disposal: Mode of disposal (e.g., incineration, release to sewage system) for each category and type of use, if appropriate; recycling possibility.

Incineration, diversion to other hydrocarbon uses.

2. Physical-Chemical Data

2.1 Melting or Decomposition Point:

Method (e.g., OECD, others): Not specified

-139.8° C

GLP: YES [ ]
NO [x]

Reference: a) Handbook of Chemistry and Physics (1985).

2.2 Boiling Point (including temperature of decomposition, if relevant):

63.3°C at 101 kPa

Method (e.g., OECD, others): Not specified

GLP: YES [ ]
NO [x]

Reference: a) Handbook of Chemistry and Physics (1985)

2.3 Density:

0.6731 g/mL @ 20°C
Solubility: very soluble in organic solvents

Reference: a) Handbook of Chemistry Physics (1985)

2.4 Vapor pressure

A. 140 mm Hg at 20°C

Method (e.g., OECD, others): Unknown

GLP: YES [ ]
NO [x]

Reference: v) Lappin,G. and Sauer, J.

B. 184 mmHg

Method: Estimated using EPIWIN

Reference: hh) USEPA EPIWIN model output for 1-hexene.
USEPA/OPPT/RAD/ECAB (8/20/99)

2.5. Partition coefficient n-Octanol/water

A. log Pow = 2.9 at (temperature not specified).

Method: calculated [x] by method of Chiou, et al., 1982
measured [ ]

GLP: Yes [ ]
No [x]

Analytical Method: N/A

Reference: b) CRCS, Inc. (1985).

B. log Pow = 3.9 at pH 6.8

Method: calculated [ ]
measured [x]

GLP: Yes [ ]
No [x]

Analytical Method: Reverse-phase HPLC (Eadsforth, 1982)

Comments (e.g., is the compound surface active or dissociative?): This result indicates a moderate potential for 1-hexene to accumulate from water into organisms.

Reference: x) Shell Research Ltd., SBGR.85.026 (1985).

C. log Pow = 3.3 at (temperature not specified).

Method: calculated [x] by method of Hansch and Leo (1979)
measured [ ]

GLP: Yes [ ] N/A
No [ ]

Analytical Method: N/A

Reference: x) Shell Research Ltd., SBGR.85.026 (1985).

D. log Pow = 3.39 at 20°C

Method: calculated [ ]
measured [x]

GLP: Yes [] Unknown [X]
No []

Analytical Method: cc) Unknown;

Comments: 3.39 was also the figure calculated utilizing USEPA's EPIWIN model.

Reference: cc) Y Tewari, J Chem. Eng. Dat 27 [1982] 451 cited in HEDSET

2.6.A Water solubility

50 mg/L at 20°C

Method (e.g., OECD, others):Not specified

GLP: YES [ ]
NO [x]

Analytical Method: Unknown

Reference: b) CRCS, Inc. (1985).

2.6 B. pH/pKa - Not available

2.7 Flash point (liquids)

-26°C [x] closed cup

Method (e.g., OECD, others including reference to the standard test used):

GLP: YES [ ]
NO [x]

Reference: c) Hazardous Chemicals Data Book (1986)

2.8 Auto Flammability: No data available

2.9 Flammability (solid/gases)

Method (e.g., OECD, others): Not specified

GLP: YES [ ]
NO [x]

Test results: LEL = approx. 2% UEL = approx. 7%

Reference: Chevron MSDS

2.10 Explosive Properties: No data available

2.11 Oxidizing Properties: No data available

2.12 Oxidation: Reduction Potential: No data available

2.13 Additional Remarks:

3. Environmental Fate and Pathways

3.1 Stability

3.1.1. Photodegradation. Stability in air (e.g., photodegradability) and in water (e.g., hydrolysis)

A. Test substance: 1-hexene

Test method or estimation method (e.g., OECD, others): Calculated but not described in detail in reference (b).

GLP YES [ ]
NO [x]

Test results: half-life with ozone = approx. 16 hrs; half life with $\overline{OH}$ = approx. 6 hrs.

Reference: b) CRCS, Inc. (1985).

B. Test substance: 1-hexene

Test method or estimation method (e.g., OECD, others): Estimated using the method of Atkinson (1985)

GLP YES [ ]
NO [x]

Test results: half-life with ozone = approx. 23 hrs; half life with $\overline{OH}$ = approx. 12 hrs.

Reference: jj) ITC, IR-427 Update, (1990 - 1991)

C. Test substance: 1-hexene

Test method or estimation method (e.g., OECD, others): Calculated using USEPA's EPIWIN model. Input values: MW=84.16; MP=-139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

GLP YES [ ]
NO [x]

Test results: half-life with ozone = approx. 23 hrs; half life with $\overline{OH}$ = approx. 4.2 hrs.

Reference: hh) USEPA EPIWIN/ECOSAR model output for 1-hexene. USEPA/OPPT/RAD/ECAB, (8/20/99)

3.1.2. Stability In Water: Hydrolysis: no data available

3.1.3 Stability in Soil:

A. Soil Adsorption

Test substance: (C_6 - C_{12}) Alpha Olefins

Test method or estimation method (e.g., OECD, others): Estimated

GLP YES [ ]
NO [x]

Test results: The C_6 - C_{12} alkenes are expected to volatize from the soil surface to the atmosphere. The high soil adsoprtion coeffecients determined for these compounds range from 3,500 to 660,000 suggesting that they will be essentially immobile in soil except when large volumes of material are present to aid in the dissolution of the alkenes (i.e. leaking underground storage tank (gasoline)). Thus, they are not expected to leach into ground water. Strong adsorption to soil may attenuate the rate at which they volatilize to the atmosphere.

Reference: jj) ITC, IR-427 Update (1990 -1991)

3.2 Monitoring data (environment)

Indicate whether the data are measurements of background concentrations or measurements at contaminated sites:

- air: 1.2 ppb (by volume) average in Leningrad as of 1977-1979

Reference: b) CRCS, Inc. (1985)

3.3 Transport and Distribution between environmental compartments including estimated environmental concentrations and distribution pathways.

3.3.1. Transport: Volatilization from Water

A. Test substance: 1-hexene
Test method or estimation method (e.g., OECD, others): Estimated

GLP YES [ ]
NO [x]

Test results: half-life = 2.7 hours from a model river 1 M deep, flowing at 1 m/sec, with a wind velocity of 3 m/sec. The volatilization from water appears to be dependent on the chain length and for a given homologous series, independent of the double bond position. Indicating volatilization from water to atmosphere to be a rapid process.

Reference: jj) ITC, IR-427-Update (1990 - 1991)

B. Test substance: 1-hexene

Test method or estimation method (e.g., OECD, others): Estimated utilizing USEPA's EPIWIN model program. Input values: MW=84.16; MP=-139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

GLP YES [ ]
NO [x]

Test results: half-life = 0.9 hours from a model river 1 M deep, flowing at 1 m/sec, with a wind velocity of 3 m/sec. Half-life = 3.6 days from a modeled lake.

Reference: hh) USEPA EPIWIN/ECOSAR model output for 1-hexene. USEPA/OPPT/RAD/ECAB (8/20/99)

3.3.2. Theoretical Distribution (Fugacity Calculations)

A. Type of transport and distribution processes between compartments (e.g., air, water, soil):

Media: air - biota - sediment(s) - soil - water
Estimation of environmental concentrations:

Results of the estimation: Input values: MW=84.16; MP=-139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

Level III Utilizing default emission values:
Air 8.5%; Water 83.1%; Soil 8.02%; Sediment 0.385%;

Level III Utilizing emission values provided by American Chemistry Council (1o kg/hr to air, 1 kg/hr to water, 0 kg/hr to soil)
Air 21%; Water 77%; Soil <1%; Sediment 2%

Level I Utilizing default emission values:
Air = 100%; Water <1%; Soil <1%; Sediment <1%
Summary of the method (or model) used: Calculation Method according to Mackay, level III [1999]

Reference: EQC model output for 1-hexene. USEPA/OPPT/EETD/EAB; David Lynch, (11/17/2000)

B. Type of transport and distribution processes between compartments (e.g., air, water, soil):

Media: air - biota - sediment(s) - soil - water
Estimation of environmental concentrations:
Results of the estimation: Input values: MW=84.16; MP=-139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

Air 100%; Water <1%; Soil <1%; Sediment <1%;

Summary of the method (or model) used: Calculation Method according to Mackay, level I [2000]

Reference: EQC model output for 1-hexene. USEPA/OPPT/EETD/EAB; David Lynch, (11/17/2000)

3.4 Mode of Degradation in Actual Use:

3.5 Biodegradation

A. Test substance: 1-hexene
Test type, aerobic [x], anaerobic [ ]
Test medium: 2 mg/L 1-hexene as emulsion in Dobane PT sulphonate solution

Test method (e.g., OECD, 150, others): Closed-bottle test 84/449/EEC

GLP YES [x]
NO [ ]

Test results: Oxidized to 22% of theoretical oxygen demand by 28 days.

Comments: No inhibition of microbial activity was detected. 1-Hexene was not "readily biodegradable."

Reference: d) Shell Research Limited (1985).

B. Test substance: 1-hexene
Test type, aerobic [x], anaerobic [ ]
Test medium: 20 mg/L 1-hexene as emulsion in Dobane PT sulphonate solution

Test method (e.g., OECD, 150, others): Modified STURM test.

GLP YES [x]

NO [ ]

Test results: 1-3% of theoretically possible CO_2 was evolved in 28 days.

Comments: No inhibition of microbial activity was detected. 1-Hexene was not "readily biodegradable."

Reference: d) Shell Research Limited (1985), SBGR 85.11.

C. Test substance: 1-hexene
Test species: Pseudomonas fluorescens

Single species tests such as "Microtox Photobacterium luminescence test" and tests on overall processes such as nitrification or soil respiration are included in this Item.

Test method (e.g., OECD, others): Microbial inhibition at 1-hexene concentrations of 10, 32, 100, 320, and 1000 mg/L (soil)

GLP YES [x]
NO [ ]

Test results: Maximum inhibition was 24% at 1000 mg/l

Comments:

Reference: d) Shell Research Limited (1985), SBGR 85.11.

D. Test Substance: 1-hexene
Test Type: Unknown
Test Media: Unknown

Test Results: Degree of Biodegradation is 67 – 98% by BOD; JETOC, No. 5, December, 1991 lists 1-hexene and 1-hexadecene among 31 readily biodegradable chemical substances as a result of testing results announced by the Japanese Ministry of International Trade and Industry (MITI) in December 1989.

Reference: w) JETOC, No.5, December 1991; MITIT, Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan (1992).

E. Test substance: 1-hexene
Test type, aerobic [x], anaerobic [ ]
Test medium:
Test method (e.g., OECD, 150, others): Estimated/Calculated using USEPA's EPIWIN model.

GLP YES [ ]
NO [X]

Test results: Aerobic: days to weeks;

Comments: Volatilization is expected to be more rapid than biodegradation.

Reference: USEPA, EAB-IRER, 1996

3.6 BOD-5, COD or Ratio BOD-5/COD: No data available

3.7 Bioaccumulation: No data available

3.8 Additional Remarks:

A. Sewage Treatment:

Test Substance: 1-hexene
Test Medium: Waste Water Treatment with a rotary disk contact aerator

Test Results: elimination of >99% of 1-hexene.

Reference: Verschueren (1983)

B. Sewage Treatment:

Test Substance: 1-hexene
Test Type: aerobic [X], anerobic [ ]
Test Medium: secondary wastewater treatment (water)

Test Method: Calculated, EPIWIN, secondary wastewater treatment removal model
Input values: MW=84.16; MP=-139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

GLP: YES [ ]
No [X]

Test Results: >99% removed from secondary wastewater treatment.

Comments: Extensive stripping to air is predicted and biodegradation potential is high.

Reference: EAB-IRER (1995), model run by USEPA/OPPT/EETD/EAB. Also, USEPA, EPIWIN; USEPA/OPPT/RAD/ECAB, (8/20/99).

C. Other: Migration to Ground Water
Test Method: Predicted using USEPA EPIWIN Input values: MW=84.16; MP=139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

Rate: moderate to rapid

Comments: may be mitigated by volatilization

Reference: EAB-IRER (1995); USEPA EPIWIN output run by USEPA/OPPT/RAD/ECAB, 8/99.

4. Ecotoxicological Data

4.1 Acute/prolonged Toxicity to Fish

A. Results of acute tests: LC_{50}(96h) >1000 mg/L (nominal concentration)

Test substance: 1-Hexene
Test species: Salmo gairdneri
Test method (e.g., OECD, others): 96 hour-static toxicity test

Type of test static [x], semi-static [ ], flow-through [ ] with daily renewal
Other (e.g., field observation) [ ]

GLP YES [x]
NO [ ]

Test results: No mortalities occurred during 96- hour exposure to 1000 mg/L 1-hexene, the highest concentration tested.

LC_{50}(96h) >1000 mg/L (nominal concentration)

Comments: the water solubility is noted to be around 46 mg/l

Reference: x) Shell Research Ltd., SBGR.85.026 (1985).

B. Test substance: 1-Hexene
Test species: Oncorhynchus mykiss

Test method (e.g., OECD, others): 96 hour semi-static toxicity test
Type of test static [ ], semi-static [x], flow-through [ ]
Other (e.g., field observation) [ ]

GLP YES [x]
NO [ ]

Test Results: The mean measured concentration of 1-hexene in the test media was approx 20 to 40% that of nominal concentrations over the first 24 hours of the test but increased to 47 to 120% for the remaining exposure periods. Based upon mean measured concentrations of 1-hexene in the test media the LC_{50} value was calculated to be:

LC_{50}(24h) = 9.7 mg/L
LC_{50}(48h) = 5.6 mg/L
LC_{50}(72h) = 5.6 mg/L
LC_{50}(96h) = 5.6 mg/L

Reference: y) Shell Research Limited, SBGR.91.252 (1991).

C. Test substance: 1-Hexene
Test species: Brachydanio rerio [zebra fish]

Test method (e.g., OECD, others): 96 hour semi-static toxicity test
Type of test static [ ], semi-static [x], flow-through [ ]

Other (e.g., field observation) [ ]

GLP YES [x]
NO [ ]

Comments: Test media were prepared by stirring with test material for 4 hr; test media were renewed daily; pH and oxygen were monitored; no chemical analyses were performed; exposure were both in open and closed containers to evaluate the role of evaporation of test material; nominal concentrations were 0, 3.2, 10, 32, 100 mg/l.

Test results: 96 hr LC50 open container est. 50 mg/l
96 hr LC50 closed container est. 25 mg/l
NOEC at 96 hr was 10 mg/l in each case

Reference: ee) Adema DMM and Bakker GH. [1985]

D. Test substance: Olefins 68 PQ11 (C_6-C_8 Cracked Wax Olefin Mixture)
$<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%

Test species: Salmo gairdneri
Test method (e.g., OECD, others): acetone used as carrier with 0.1 ml/L with appropriate control

Type of test: static [X], semi-static [ ], flow-through [ ]
Other (e.g., field observation) [ ]

GLP: YES [X]
NO [ ]

Test results: LC50 (96hr) = 100 mg/l (nominal)

Comments:
Reference: Shell Research Limited Group Research Report: SBGR.83.357

E. Test substance: 1-hexene
Test method: USEPA EPIWIN/ECOSAR Input values: MW=84.16; MP=-139.7C; BP=63.4C; WS=50 mg/L; VP=184 mmHg

Test Species: Fish (freshwater)
Test Results: LC50 (96 hr) = 3.080 ppm, LC50 (14 day) = 6.957 ppm,

Test Species: Saltwater Fish
Test Results: LC50 (96-hr) = 1.382 ppm

Reference: hh) USEPA EPIWIN/ECOSAR model output for 1-hexene. [8/20/99]

4.2 Acute Toxicity to Aquatic Invertebrates - daphnids

A. Test substance: 1-Hexene
Test species Daphnia magna

Test method (e.g., OECD, others): 48-hour static toxicity test

GLP YES [x]
NO [ ]

Test results: EC_{50} (48h) 230mg/L (determined concentration)

The 24- and 48-hour EC_{50} values were calculated to be 540 mg/L of 1-hexene and 230 mg/L (95% fiducial limits 190-280 mg/L) respectively.

Comments: The results reported are considered nominal, since they are above the water solubility of the test substance. No precautions were taken to prevent evaporative losses from the test vessels.

Reference: x) Shell Research Ltd., SBGR.85.026 (1985).

B. Test substance: 1-Hexene
Test species Daphnia magna

Test method (e.g., OECD, others): 48-hour static toxicity test

GLP YES [x]
NO [ ]

Test results: 48 hr LC50 open container est. 60 mg/l
NOEC after 48 hr was 32 mg/l
48 hr LC50 closed container est. 30 mg/l
NOEC after 48 hr was 10 mg/l

Comments: test media were prepared by stirring with test material for 4 hr; test media were not renewed; pH and oxygen were monitored; no chemical analyses were performed; exposure were both in open and closed containers to evaluate the role of evaporation of test material; nominal concentrations were 0, 3.2, 10, 32, 100 mg/l.

Reference: ee) Adema DMM and Bakker GH. [1985]

C. Test substance: Olefins 68 PQ 11 (C_6- C_8 Cracked Wax Olefins Mixture)
$<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%

Test species: Daphnia Magna
Test method (e.g., OECD, others): Static; acetone used as carrier to 0.1 ml/L with appropriate control
GLP: YES [ ]
NO [X]

Test results: EC50 (48hr) = 67 mg/l (nominal)

Comments:

Reference: Shell Research Limited Group Research Report SBGR.83.357.

D. Test substance: 1-hexene
Test method: Predicted by EPA EPIWIN/ECOSAR model (input) Log Kow = 3.39, Water solubility = 50 mg/L, MW = 84.16.

Test Species: Daphnia
Test Results: LC50 (48 hr) = 3.633 ppm,

Test Species: Green Algae
Test Results: EC50 (96 hr) = 2.460 ppm,

Test Species: Fish
Test Results: LC50 (96 hr) = 3.080 ppm, LC50 (14 day) = 6.957 ppm, ChV (30 day) = 0.496 ppm

Reference: hh) USEPA EPIWIN/ECOSAR model output for 1-hexene. [8/20/99]

4.3 Toxicity to Aquatic Plants (eg. algae):

A. Test substance: 1-Hexene (Shop C6 Linear Alpha Olefin)
Test species: Selenastrum capricornutum
Test method (e.g., OECD, others): 4-day growth experiment

GLP YES [x]
NO [ ]

Test results:

EC50 (96h) = >1000 mg/L (nominal concentration) (author assigned)
EL0 (96h) = >22 mg/L*

Comments: The highest nominal concentration of 1-hexene tested, 1000 mg/L, did not cause reduction in cell numbers at day 4 compared to the mean cell number at day 4 in the controls.

*Upon review of the study it was noted that five concentrations were tested above the water solubility of Shop C6 Alpha Olefin (1-hexene). In light of those concentrations being above the water solubility it was determined to assign the EL0 (96h) with a value of > 22 mg/L. 22 mg/L was the highest nominal concentration below the water solubility at which the substance was tested. EL0 = effect loading based on WAF testing procedure; no effect observed at the highest loading indicated.

Reference: x) Shell Research Ltd., SBGR.85.026 (1985).

B. Test substance: Olefins 68 PQ 11 (C_6-C_8 Cracked Wax Olefins Mixture)
$<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%

Test species: Selenastrum capricornutum
Test method (e.g., OECD, others): 4-day Growth Method
GLP: YES [X]
NO [ ]

Test results: EC50 (96hr) = 200 mg/l
Comments:
Reference: Shell Research Limited Group Research Report SBGR. 83.357.

C. Test substance: 1-hexene

Test method: Predicted by EPA EPIWIN/ ECOSAR model (input) Log Kow = 3.39, Water solubility = 50 mg/L, MW = 84.16.

Test Species: Green Algae
Test Results: EC50 (96 hr) = 2.460 ppm,

Reference: hh) USEPA ECOSAR model output for 1-hexene. [8/20/99]

4.4 Toxicity to Bacteria:

A. Test substance: 1-hexene
Test species: Mixed marine bacterial culture.

Single species tests such as "Microtox Photobacterium luminescence test" and tests on overall processes such as nitrification or soil respiration are included in this Item.

Test method (e.g., OECD, others): Acute static bioassay (Aquatic)

GLP YES [ ]
NO [X]

Test results: Toxic effect with a log EC10 of -0.49 mg/L. However, the calculated log LC50 was 0.46, indicating a value > 100% saturation in sea water.

Comments: 1-hexene was designated not toxic up to levels of 100% saturation in sea water.

Reference: f) Warne, et al. (1989)

4.5 Chronic Toxicity to Aquatic invertebrates:

Test substance: 1-hexene
Test method: Predicted by EPA EPIWIN/ECOSAR model (input) Log Kow = 3.39, Water solubility = 50 mg/L, MW = 84.16.

Test Species: Daphnia
EC50 (16 day) = 0.342 ppm

Test Species: Green Algae
ChV (96 hr) = 0.549 ppm

Test Species: Fish (freshwater)
LC50 (14 day) = 6.957 ppm, ChV (30 day) = 0.496 ppm

Reference: hh) USEPA EPIWIN/ECOSAR model output for 1-hexene. [8/20/99]

4.6 Toxicity to Terresterial Organisms: No data available

4.6.1. Toxicity to soil dwelling Organisms: No data available

4.6.2. Toxicity to terrestrial plants: No data available

4.6.3 Toxicity to birds: No data available

5. Toxicological Data

5.1 Acute toxicity

5.1.1 Acute oral toxicity

Test substance: 1-hexene
Test species/strain: rat/F344
Test method (e.g., OECD, limit test, fixed dose test): OECD 401

GLP YES [x]
NO [ ]

Test results: No deaths in 5 males or 5 females at 5.6 g/kg
(LD50 > 5.6 g/kg); no treatment-related gross pathology

Discriminating dose (for fixed dose only): 5.6 g/kg

Comments: An earlier test (Reference h) resulted in no deaths at 10 g/kg in 10 male Wistar rats

Reference: g) Shell Development Company (1982).
h) Rinehart, (1967).

5.1.2 Acute inhalation toxicity

Test substance: 1-hexene
Test species/strain: rat/Wistar, 10 males/group

Test method (e.g., OECD, EC, limit test): 4-hr. exposures to seven different concentrations in a dynamic exposure system. Survivors observed for 14 days.

GLP YES [ ]
NO [x]

Test results:
Concentration: 0, 27600, 28600, 30500, 33200, 37000, 41200 ppm
Mortality: 0, 0 2 5 7 8 10/10

No treatment-related gross pathology

LC50: 32,000 ppm

Comments: Reported vapor concentrations were nominal values based on the total airflow and the weight loss of the vapor generator. Vapor concentration values obtained with a calibrated combustible gas analyzer were similar to or slightly greater than the nominal values.

Reference: h) Rinehart (1967).

5.1.3 Acute dermal toxicity

Test substance: 1-hexene
Test species/strain: albino rabbits/New Zealand white
Test method (e.g., OECD, limit test): OECD 402 [except that four males and four females were listed]

GLP YES [x]
NO [ ]

Test results: No deaths or signs of systemic toxicity at 2.0 g/kg; no treatment-related gross pathology except at application site.
LD50: >2.0 g/kg

Comments: An earlier study (Reference h) indicated no lethality nor systematic toxicity in four male rabbits after treatment at 10 g/kg.

Reference: i) Shell Development Company (1982).

5.2 Corrosiveness/Irritation

5.2.1 Skin Irritation

A. Test substance: 1-hexene
Test species/strain: 6 rabbits/New Zealand White

Test method (e.g., OECD, others): OECD 404 except that the exposure was 24 hours and skin was evaluated only at 24 and 72 hours.

GLP YES [x]
NO [ ]

Test results: The maximum score for any animal was at 24 hours and was 2 for erythema and 0 for edema. The Draize primary irritation score (range 0 - 8.0) was 0.975.

Reference: j) Shell Development Company (1982)

B. Test substance: 1-hexene (Shop Olefin C_6) : >99% 1-hexene
Test species/strain: 3 male and 3 female/New Zealand White Rabbits

Test method (e.g., OECD, others): 4 hr skin irritancy

GLP YES [ ]
NO [X]

Test results: 4 hour skin irritancy observed at 24, 48 and 72 hours was 0 for erythema and edema.

Reference: Shell (1985); SBGR 85.166, “Toxicology of Shop Olefin: The Skin Irritancy of Shop Alpha Olefin C_6; C_{18}; and Shop Olefins 103.

C. Test substance: 1-hexene
Test species/strain: New Zealand White
Test method (e.g., OECD, others

GLP YES [ ]
NO [X]

Test Results: Draize Score 1.0

Reference: h) Rinehart 1967

Classified as non-irritating by US OSHA and EU criteria

5.2.2. Eye Irritation

A. Test substance: 1-hexene
Test species/strain: albino rabbits/New Zealand white
Test method (e.g., OECD, others):OECD 405, 3 male and 3 female - unwashed; 3 males - washed.

GLP YES [x]
NO [ ]

Test results: The maximum total Draize score for any animal was 8 at 1 hour. The average total Draize score (range 0 - 110) occured at 1 hour, and was 5.0 for unwashed and 5.3 for washed eyes - “mildly irritating”.

Comments: Washing did not reduce irritation.

Reference: k) Shell Development Company: (1982)

B. Test substance**:** 1-hexene
Test species/strain: albino rabbits/New Zealand white

Test method (e.g., OECD, others):

GLP YES [ ]
NO [X]

Test results: No corneal opacity or iritis. Draize score 1.7/110.

Reference: h) Rinehart 1967

5.3. Skin sensitization

Test substance: 1% w/w 1-hexene in ethanol
Test species/strain: Guinea pig/Duncan-Hartley albino

Test method (e.g., OECD, others): OECD 406 - Buehler

GLP YES [x]
NO [ ]

Test results: Negative for sensitization
Number of animals with skin reaction at challenge: 0/10
Number of animals with skin reaction in control group at challenge: 0/10

Comments: DNCB was used as a positive control

Reference: 1) Shell Developmental Co. (1982)

5.4. Repeated Dose

A. Inhalation repeated dose

Test substance: Neodene ®6, (90 – 100% 1-hexene)
Test species/strain: rat/F344 40 males, 40 females per group

Test method (e.g., OECD, others): Protocol WTP-207, OECD Test Method 413: OECD 413 - 90 days (6 hr/day, 5 day/week, 13 weeks) to 0, 300, 1000, 3000 ppm.Ten rats/sex/group interim sacrifice at 7 weeks.

Another 10 rats/sex/group evaluated weekly for neuromuscular coordination using a rotorod.

GLP YES [x]
NO [ ]

Test results: No mortalities and no treatment-related clinical signs of toxicity 3000 ppm females had significantly lower body weights.

Clinical pathological changes which may be treatment-related included: elevated serum phosphorus in males at 300, 1000 and 3000 ppm and in females at 1000 and 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.

3000 ppm males had higher relative and absolute testes weights. No treatment-related gross or histological lesions were noted in these or other tissues at either the interim or terminal sacrifice. Sperm counts were observed and not considered to show statistical significance. (Please see Reproductive/Developmental Toxicity section 5.8.1 for further details)

There was no effect on neuromuscular performance.

The no observed adverse effect level appeared to be 1000 ppm, based on changes in body weight and questionable organ weight changes at 3000ppm.

Reference: m) Shell Development Co. (1984)

B. Repeated dose toxicity (gavage)
Test substance: 1-hexene
Test species/strain: rat/Wistar

Test method (e.g., OECD, others): OECD Test Method 407 [1981]: Groups of 5 male and 5 female rats were doses daily for 28 days with undiluted 1-hexene; controls were dosed with water. Dose levels were 10, 101, 1010, and 3365 mg/kg/day.

GLP YES [x]
NO [ ]

Test results: The main effect of dosing was irritation of the gastric mucosa, as observed by macro- and microscopic examination at the top two dose levels. Body weights were reduced at these doses. Clinical signs of hunched posture and ruffled fur were seen at the top dose, probably reflecting general discomfort. Spleen weights were reduced at the top dose, but there were no associated histological findings. Opthalmoscopy, clinical chemistry, hematology, and neuromuscular coordination [by rotorod] were unaffected. Pathological changes were restricted to gastric effects. The NOEL was 101 mg/kg.

Comments: A subsequent 13 week study was initiated but was not finalized due to unacceptably high mortality as a consequence of accidental introduction of undiluted 1-hexene into the lungs during the gavage dosing, or aspiration.

Reference: aa) Dotti et al 1994 cited in HEDSET

5.5 Genetic toxicity

A. Bacterial test

a. Test substances: 1-hexene in ethanol
Test species/strain: S. typhimurium TA98, TA100, TA1535, TA1537, TA 1538

Test method (e.g., OECD, others): OECD 471 without repeat assay

GLP YES [x]
NO [ ]

Test results: Minimum concentration of test substance at which toxicity to bacteria was observed:

with metabolic activation: 0.5 mg/plate
without metabolic activation: 0.5 mg/plate

Concentration of the test compound resulting in precipitation: none observed

Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[x]
without metabolic activation:	[ ]	[ ]	[x]

Comments: Tested from 0.002 to 0.5 mg/plate

Reference: n) Shell Development Company (1982)

b. Test substance: 1-hexene in ethanol
Test species/strain: S. typhimurium TA98, TA100, TA1535, TA1537, TA1538

Test method (e.g., OECD, others): OECD 471 with repeat assay

GLP YES [x]
NO [ ]

Test results: Minimum concentration of test substance at which toxicity to bacteria was observed:

with metabolic activation: 5 mg/plate (all strains); 0.5 mg/pl (TA98)
without metabolic activation: 0.5 mg/plate

Concentration of the test compound resulting in precipitation:
Not reported in summary

Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[x]
without metabolic activation:	[ ]	[ ]	[x]

Comments: Tested from 0.0015 to 0.5 mg. per plate

Reference: o) Huntingdon Research Center (1990)

B. Non-bacterial in vitro test

a. Test substance: 1-hexene in ethanol
Type of cell used: Chinese hamster ovary (CHO)

Test method (e.g., OECD, others): OECD 473 - Chromosome aberration (duplicate assay but not with duplicate cultures, cells evaluated at 12 hours)

GLP: YES [x]
NO [ ]

Test results: Lowest Concentration producing cell toxicity:
with metabolic activation: 0.61 mg/l
without metabolic activation: 0.067 mg/l

Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[x]
without metabolic activation:	[ ]	[ ]	[x]

Comments: A single increase in aberrations was noted in the first assay (with S-9) but was not dose-related or reproduced in the second assay. There was no evidence that the cell cycle was not delayed.

Reference: p) Shell Development Company (1983)

b. Test substance: 1-hexene in 7.5% Pluronic F68 Polyol
Test species/strain: Primary rat hepatocytes

Test method (e.g., OECD others): OECD 482 - unscheduled DNA synthesis (UDS), no confirmatory assay.

GLP: YES [x]
NO [ ]

Test results:

Lowest Concentration producing cell toxicity:
56.7% viability at 5 mg/mL
77% viability at 2.048 mg/mL

Genotoxic effects: Negative at 0.5 and 2.0 mg/mL; no evaluation at 3.5 and 5.0 mg/mL due to toxicity.

Comments: Positive control produced expected results.

Reference: q) Gulf Life Sciences (1984)

c. Test substance: 1-hexene (solvent unknown)
Type of cell used: Mouse lymphoma L51784

Test method (e.g., OECD, others): Mammalian Cell Gene Mutation TK+/-)

GLP: YES [x]
NO [ ]

Test results:
Lowest Concentration producing cell toxicity: Not reported in summary.
Genotoxic effects: Negative with and without S-9

Comments:

Reference: r) Huntingdon Research Center (1990)

d. Test substance: 1-hexene (solvent unknown)
Type of cell used: Cultured human lymphocytes

Test method (e.g., OECD, others): Metaphase chromosome analysis

GLP: YES [x]
NO [ ]

Test Results:
Lowest Concentration producing cell toxicity: Not reported in summary.
Genotoxic effects: Negative with and without S-9

Comments: Test concentrations were 15.6, 62.5 and 125 mg/mL

Reference: s) Huntingdon Research Center (1990)

e. Test substance: Gulftene 6 [1-hexene]; solvent Pluronic F68 [10% aq.]
Type of cell used: BALB/3T3 Transformation Assay

Test method (e.g., OECD, others):

GLP: YES [ ]
NO [X]

Test Results: negative
Lowest Concentration producing cell toxicity: 32 ug/ml; concentrations of 32 - 5000 ug/ml were cytotoxic

Comment: For cell transformation testing, concentration range was 256-2048 ug/ml.

Reference: gg) Goode and Brecher 1983.

5.6. Non-bacterial test in vivo

Test substance: 1-hexene
Test species/strain: mice/Cr1:CD-1 (ICR) BR

Test method (e.g., OECD, others): OECD 474 - micronucleus. Mice exposed to 0, 1000, 10000, or 25000 ppm 2 hrs/day for 2 days. Bone marrow smears examined for micronucleated polychromatic erythrocytes. Cyclophosphamide positive control.

GLP: YES [X]
NO [ ]

Test results: Lowest doses producing toxicity: 10,000 ppm (transient lethargy)
Effect on Mitotic Index or P/N Ratio: Equivocal on day 3.

	+	?	-
Genotoxic effects:	[ ]	[ ]	[x]

Reference: t) Gulf Life Sciences (1983)

5.7 Carcinogenicity: No data available

5.8 Toxicity to Reproduction

5.8.1. Reproductive Toxicity (inhalation)

A. Test substance: 1-hexene
Test species/strain: rat/F344 40 males, 40 females per group

Test method (e.g., OECD, others): OECD Test Method 413 - 90 days (6 hr/day, 5 day/week, 13 weeks) to 0, 300, 1000, 3000 ppm. Ten rats/sex/group interim sacrifice at 7 weeks.

Another 10 rats/sex/group evaluated weekly for neuromuscular coordination using a rotorod.

GLP YES [x]
NO [ ]

Test results:
General Toxicity: Please see Repeated Dose Section 5.4.1 for details.

Reproductive Toxicity: At terminal sacrifice, there appeared to be a dose-related increase in testes weight which was statistically significant at the highest exposure concentration of 3000 ppm (see page 189 of the original study). This increase in testes weight did not appear to be accompanied by any

histopathology nor any apparent effect on sperm count. Sperm morphology and motility were not evaluated. An increase in sperm counts and testis weight in all animals at terminal sacrifice was observed when compared to the interim sacrifice (page 121 vs 189 in the original study), however, the increase considered to be attributed to the increase in age of the animal. Since testes weight measurements in and of themselves do not indicate the exact nature of an effect, a significant increase or decrease is indicative of an adverse effect. In this case, there was no histopathology and the sperm counts were within control range. However, damage to the testes may be detected as a weight change only at doses higher than those required to produce significant effects in other measures of gonadal status and it appears that only a minimal evaluation of gonadal status was conducted in this 90-day study. As a result the significance of increases in testes weight is unclear.

The NOEL for reproductive effects from the limited data in the 90-day study appears to be at the mid-concentration of 1000 ppm.

Reference: m) Shell Development Co. (1984) (ii) USEPA review (1999)

B. Test substance: 1-hexene; three test articles were blended to produce the final test article consisting of 90-100% hexene. Neodene 6, Gulftene 6 and alpha olefin 6.

Test species/strain: rat; Sprague-Dawley, male and female

Test method (e.g., OECD, others): OECD 421 [modified]. Male rats were exposed for 28 days prior to mating, and through mating until euthanasia for a total of 44 consecutive days of dosing; females were dosed for 14 days prior to mating, during mating, gestation and lactation through euthanasia at lactation day 4 [41-55 consecutive days]. Dose levels were 0, 100, 500, 1000 mg/kg/day in a corn oil vehicle [5 mL/kg].

GLP: YES [x]
NO [ ]

Test results:
NOEL for P generation; females >1000 mg/kg; males < 100 mg/kg [kidney histopathology]
NOEL for F1 generation; > 1000 mg/kg/day
NOEL for F2 generation; not applicable
Maternal and Paternal general toxicity: see Comments
Reproductive toxicity observed in parental animals (fertility, gestation, reproductive organ toxicity, etc.): none
Reproductive toxicity observed in offspring ; (weights of litter, postnatal growth, viability, etc.): none

Comments: 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 behaviour. There was no evidence of developmental toxicity in the F1 generation, as measured by 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.
No mortality or clinical signs of toxicity were observed. For the F0 males and females at the top dose, gross and histological examination of the ovaries , testes, epididymides, liver, kidneys , and peripheral [sciatic] nerve was performed; kidneys were also examined at the mid and low dose levels. The only gross finding was pitted kidneys in a few mid and top dose males, and the only histological finding was dose-related accumulations of hyaline droplets in the epithelial cells of the convoluted tubules of the kidneys of males; no such effect was observed in female rats. This condition was diagnosed as hydrocarbon nephropathy, which is considered specific to young adult male

rats; there is no indication that similar nephropathy will occur in humans exposed to 1-hexene.

Reference: dd) EM Daniel [1995]

5.9. Teratogenicity/Developmental toxicity: Please see Section 5.8.

5.10. Specific toxicities (Neurotoxicity, immunotoxicity etc.)

If ingested, 1-hexene may be readily aspirated into the lungs if vomiting occurs. Chemical pneumonitis may occur.

Reference : bb) Gerarde and Linden [1963]

Neurobehavioral toxicity was evaluated in a 90-day inhalation study (see 6.4)

5.11. Experience with human exposure

A. In a review, Cavender (1994) noted that 1-hexene, when inhaled, may produce narcosis in humans at a concentration of 0.1 percent with accompanying CNS effects, mucous membrane irritation, vertigo, vomiting and cyanosis.

Reference: Cavender, F.; Patty's Industrial Hygiene and Toxicology, 4th ed, Vol 2, Part B, Chapter 19, pgs 1221-1249, Aliphatic Hydrocarbons

B. Chevron (19840 reported that prolonged or frequently repeated contact with (C_6 – C_{12}) alkenes may cause the skin to become dry or cracked from the defatting action of the compounds. Breathing of vapor of (C_6 – C_{12}) alkenes may cause CNS depression. Signs and symptoms of CNS depression may include one or more of the following: headache, dizziness, loss of appetite, weakness and loss of coordination. Affected persons usually experience complete recovery when removed from the exposure area.

Reference: b) CRCS [1985]

5.12 Toxicodynamics, toxico-kinetics

A. NEODENE 6 alpha olefin (1-hexene) was tested in an in vitro system and was demonstrated to cause the autocatalytic ("suicidal") destruction of cytochrome P-450 and heme in hepatic microsomes ffrom phenobarbital pretreated rats. The destructive process was time dependent, saturable and required NADPH. Destruction was inhibited by metyrapone and carbon monoxide but not by glutathione. Reduced oxygen tension did not prevent the loss of cytochrome P-450. NEODENE 6 alpha olefin was shown to be a substrate for cytochrome P-450 by its binding spectrum to the cytochrome.

Reference: u) Shell Development Company (1984)

B. Some olefins have been shown to be metabolized to epoxides. For example, ethylene and propylene have been shown to be metabolized to their corresponding oxides by the presence in animals of the corresponding hemoglobin and DNA adducts. Absorption, distribution, elimination and hemoglobin and DNA adduct formation were studied in the rat after inhalation of individual C_2 - C_8 1-alkenes [including 1-hexene] at 300 ppm, 12 hr /day for 3 consecutive days. Concentrations of olefins were measured in blood and organs reached steady state levels after the first 12 hr of exposure, and the concentrations 12 hr after the last exposure were generally low, except in the fat. Concentrations of 1-alkenes in blood and tissues increased with increasing number of carbon atoms. In contrast, levels of hemoglobin and DNA adducts

decreased with increasing number of carbon atoms. The decrease was most pronounced from C2 to C3.
Reference: ff) Eide I et al., 1995

Comment: The increased retention in fat of 1-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 1-alkenes. Since unchanged 1-alkenes are not considered to be toxic, and because tissue levels rapidly cleared after exposure ceased, this concentration especially in fat tissues is unlikely to have any biological effect. An implication of the metabolic formation of an epoxide, as determined by hemoglobin and DNA adducts, is that the 1-alkenes are likely to be genotoxic. However ethylene, which formed these adducts to a much greater extent than the higher homologs, has been specifically investigated in lifetime animal cancer bioassays at concentrations up to 3000 ppm, and determined to be negative [Guest et al., 1984]. It is highly unlikely that the higher homologs, including 1-hexene, will be genotoxic or carcinogenic under these conditions.

6. REFERENCES:

a) Handbook of Chemistry and Physics, 65th ed., CRC: Boca Raton, FL, 1985; page C-331.

b) CRCS, Inc.: Information Review (C_6 - C_{12}) Alkenes, IR-427, Prepared under EPA Contract No. 68-01-6650; Rockville, MD, 1985.

c) Hazardous Chemicals Data Book, 2nd ed., Weiss, G. Ed.: Noyes Data Corp., Park Ridge, NJ, 1986.

d) Shell Research Limited: "Shop C_6 Alpha Olefins: An Assessment of Ready Biodegradability", Document SBGR.85.111, April 1985 (unpublished report).

e) Verschueren, K.: Handbook of Environmental Data on Organic Chemicals, 2nd ed., Van Nostrand Reinhold Company, New York, NY, 1983.

f) Warne, M.St.J., Connell, D.W., Hawker, D.W., and Schuurmann, G.: Quantitative Structure-Activity Relationships for the Toxicity of Selected Shale Oil Components to Mixed Marine Bacteria. Ecotoxicol. Environ. Safety 17:133-148, 1989.

g) Shell Development Company: "Acute Oral Toxicity of NEODENE 6 Alpha Olefin in the Rat:, WTP-120, March 1982 (unpublished report).

h) Rinehart, W.E.: "Toxicological Studies on Several Alpha Olefins", University of Pittsburgh, June, 1967, submitted to Gulf Research and Development Co., (unpublished report).

i) Shell Development Company: "Acute Dermal Toxicity of NEODENE 6 Alpha Olefin in the Rabbit:, WTP-124, March 1982 (unpublished report).

j) Shell Development Company: "Primary Skin Irritation of NEODENE 6 Alpha Olefin in the Rabbit", WTP-121, March 1982 (unpublished report).

k) Shell Development Company: "Eye Irritation of NEODENE 6 Alpha Olefin in the Rabbit", WTP-122, March 1982 (unpublished report).

l) Shell Development Company: "Guinea Pig Skin Sensitization of NEODENE 6 Alpha Olefin", WTP-123, March 1982 (unpublished report).

m) Shell Development Company: "90-Day Vapor Inhalation Study in Rats with NEODENE 6 Alpha Olefin", WTP-207, July 1984 (unpublished report.

n) Shell Development Company: "Gene Mutation in Salmonella typhimurium Assay of NEODENE 6 Alpha Olefin", WTP-136, March 1982 (unpublished report).

o) Huntingdon Research Center: "1-Hexene: Bacterial Mutation Assay", Sept. 1990, sponsored by Ethyl (unpublished report).

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

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

r) Huntingdon Research Center: "1-Hexene in Vitro Mammalian Cell Gene Mutation Assay (TK+/-)", Sept. 1990, sponsored by Ethyl (unpublished report).

s) Huntingdon Research Center: "1-Hexene: Metaphase Chromosome Analysis of Human Lymphocytes Cultured in Vitro", Sept. 1990, sponsored by Ethyl (unpublished report).

t) Gulf Life Sciences: "Micronucleus Test in Mouse Bone Marrow: GULFTENE 6 Administered by Inhalation Using 2 Daily 2-Hour Treatments", project #82-119, July 1983 (unpublished report).

u) Shell Development Company: "In Vitro Destruction of Hepatic Cytochrome P-450 and Heme by NEODENE 6 Alpha Olefin", WRC-814, March 1984 (unpublished report).

v) Lappin, George R., Sauer, Joe D. Alpha Olefins Applications Handbook, Marcel Dekker, Inc., New York.

w) Japan Chemical Industry Ecology-Toxicology and Information Center, (JETOC, No. 5, December 1991) "Biodegradation and Accumulation Testing Results on Existing Chemical Substances."

x) Shell Research Limited, SBGR.85.026, "Shop C_6 Linear Alpha Olefins (1-Hexene); Acute Toxicity (Salmo gairdneri, Daphnia magna and Selenastrum capricornutum) and N-Octanol/Water Partition Coefficient", January 1985.

y) Shell Research Limited, SBGR.91.252, "1-Hexene: Acute Toxicity to Oncorhynchus mykiss", November 1991.

z) D Mackay. [1991]. Multimedia Environmental Models: The fugacity approach. Lewis publishers Inc. Chelsea Michigan USA, 1991 Chapter 5. cited in HEDSET

aa) Dotti A, Dubach-Powell, JR, Biederman K, Weber K. 4-Week Oral Toxicity (gavage) Study with 1-Hexene in the Rat. RCC Project 332695. Cited in HEDSET.

bb) Gerarde HW and Linden NJ [1963] Toxicological Studies on Hydrocarbons. Archives of Environmental Health, 6, p35-47.

cc) Y Tewari, J Chem. Eng. Dat 27 [1982] 451 cited in HEDSET

dd) EM Daniel. Reproduction/Developmental Toxicity Screening Test In Rats with 1-Hexene. Springborn Laboratories. Sponsored by Chemical Manufacturers Association [1995]

ee) Adema DMM and Bakker GH. Aquatic toxicity of compounds that may be carried by ships [MARPOL 1973; Annex II]. TNO report R 85/217, The Hague [1985]

ff) Eide I, Hagerman R, Zahlsen K et al;, Uptake, distribution, and formation of hemoglobin and DNA adducts after inhalation of C2-C8 1-alkenes [olefins] in the rat. Carcinogenesis. 16, 1603 - 1609 [1995]

gg) Goode JW and Brecher S. Unpublished report by Gulf Life Sciences Institute, Pittsburg PA 1983

hh) USEPA ECOSAR model output for 1-hexene. Amuel Kennedy [8/20/99]

ii) USEPA review of Shell, 1984 90-day Inhalation study conducted by Katherine Anitole [8/26/99]

jj) ITC, IR-427 Update (1990 - 1991)

kk) Cavender, F.; Patty's Industrial Hygiene and Toxicology, 4th ed, Vol 2, Part B, Chapter 19, pgs 1221-1249, Aliphatic Hydrocarbons

ll) EQC model output for 1-hexene. USEPA/OPPT/EETD/EAB; David Lynch, (11/17/2000).

1- OCTENE (CAS N°: 111-66-0)

FULL SIDS SUMMARY

CAS NO.: 111-66-0		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point	N/A	N/A	-101.73°C
2.2	Boiling Point	N/A	N/A	121-123°C at 1atm. (5% and 95%)
2.3	Density	N/A	N/A	714.9 kg/m^3
2.4	Vapour Pressure	N/A	Measured Calculated	20.3 hPa at 20°C (15.23 mmHg) 23.2 hPa at 25°C (calculated)
2.5	Partition Coefficient (Log K_{ow})	N/A	C_{6-8}AO: (a) calculated (b) measured	 (a) log P_{ow} = 4.4 - 5.5 (at pH 6.7) (b) log P_{ow} = 3.5 - 4.6
2.6	Water Solubility	N/A	Measured	4.1 mg/l at 25°C; Practically Insoluble
	pH and Pka values	-----	-----	N/A
2.7	Flash Point		Closed Cup	10°C (measured) ; 21°C (Aldrich
2.12	Oxidation: Reduction Potential	-----	-----	N/D
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation	N/A	Calculated	In air $T_{1/2}$ = 3.8 hours (hydroxy radical) $T_{1/2}$ = 22 hours (ozone)
3.1.2	Volatilization from Water	-----	Calculated	$T_{1/2}$ (river) = 1 hr $T_{1/2}$ (lake) = 4 days
3.1.3	Soil Adsorption	-----	Estimated C_8	K_{oc} = 507
3.2	Monitoring Data	-----	-----	(1) Air ≈ 23 tons/year; (2) Water < 1 ton/year; (3) Organic Waste ≈ 1 ton/year.
3.3	Transport and Distribution		Calculated Mackay Level III Fugacity Level I	In Air 15 % In Water 61 % In Soil <1 % In Sediment 23 % In Air 99.97%
3.5	Biodegradation	N/D	Calculated/Predicted	Days to weeks – Volatilization is expected to be more rapid than biodegradation.
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Rainbow Trout (Salmo gairdneri) Zebra Fish (*Brachiodanio Rerio*) Zebra ra Fish (*Brachiodanio Rerio*)	C_{6-8} AO blend*: Static 96-hr Static Test (beaker covered with watch glass) 96-hr Static Test (stoppered flask)	LC_{50} (96 hr) = 100 mg/l LC_{50} (24 hr) = 10 mg/l (nom.), LC_{50} (48 hr) = 4.8 mg/l (nom.), LC_{50} (72 hr) = 4.8 mg/l (nom.), LC_{50} (96 hr) = 4.8 mg/l (nom.) LC_{50} (24 hr) = >3.2<10 mg/l (nom.) LC_{50} (48 hr) = >3.2<10 mg/l (nom.) LC_{50} (72 hr) = >3.2<10 mg/l (nom.) LC_{50} (96 hr) = >3.2<10 mg/l (nom.)

CAS NO.: 111-66-0		**SPECIES**	**PROTOCOL**	**RESULTS**
		Fresh water	Predicted	96-hr LC_{50} =0.31 mg/L
		Salt water	Predicted	96-hr LC_{50} =0.25 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	Daphnid (*Daphnia magna*)	C_{6-8}AO blend*: 48-hr Static Test	24-hr EC_{50} = 85 mg/L 48-hr EC_{50} = 67 mg/L
			48-hr Static Test (beaker covered with watch glass; also stoppered flask)	48-hr EC_{50} >3.2 <10 mg/L NOEC (48 hr) = 3.2 mg/l
			Predicted	48-hr EC_{50} = 0.40 mg/L
4.3	Toxicity to Aquatic Plants	Algae (*Selenastrum capricornutum*)	C_{6-8}AO blend*:4-Day Growth Test	96-hr EC_{50} =200 mg/l
		Green Algae	Predicted	96-hr EC_{50} = 0.30 mg/l
		Green Algae	Predicted	96-hr MATC(ChV) = 0.131 mg/L
4.5.1	Chronic Toxicity To Fish	Fish (freshwater)	Predicted	30-day = 0.06 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	Daphnid	Predicted	16-day EC_{50} = 0.07 mg/l
4.6.1	Toxicity to Soil Dwelling Organisms (Bacteria)	(*Pseudomonas fluorescens*)	Microbial Inhibition Test	IC_{50} (6h) >370 mg/l
4.6.2	Toxicity to Terrestrial Plants	-----	-----	N/D
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (including Birds)	-----	-----	N/D
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	measured;	LD_{50} >10 g/kg
			measured	LD_{50} > 5 ml/kg
5.1.2	Acute Inhalation Toxicity	Rat	N/D	4-hr LC_{50} = 8,050 ppm
5.1.3	Acute Dermal Toxicity	Rabbit	measured; C_{6-8}AO blend*	LD_{50} >10 g/kg (24 hr exposure)
			measured	LD_{50} = 1.43 g/kg (24 hr exposure)
5.2.1	Skin Irritation	Rabbit	FHSA Method	PII = 1.8/8.0 (24-hr exposure)
			FHSA Method (occluded)	PII = 3.38/8.0 (24-hr exposure)
			OECD 404	PII = 3.42/8.0 (4-hr exposure)
5.2.2	Eye Irritation	Rabbit	FHSA Method	All scores zero except one conjunctival score of 2 at 24-hrs.
			FH FHSA Method	Mean Draize = 3.0 at 1-hr; 0.3 at 24-hr; 0.0 thereafter. 4.7/110 (washed) after 1 hr exposure.
5.3	Skin Sensitization	Guinea Pig	Buehler Method - OECD 406	Negative - Not a skin sensitizer
5.4	Repeated Dose Toxicity	Rabbit	28-Day Skin Irritation	Treated animals had questionable hyperemia, questionable exfoliation, and questionable scab formation at the end of the study.
		Rat	90-day Oral (gavage) dosing at 0, 5, 50 or 500 mg/kg/bw for 7	(NOEL) = 50 mg/kg/bw/day. Slight changes at highest dose level, to include increased kidney weights and

CAS NO.: 111-66-0		SPECIES	PROTOCOL	RESULTS
			days/week for 13 weeks.	decreased plasma chloride in both sexes, increased urinary volume and unspecified microscopic kidney differences in male rats only, and increased creatinine in females only.
5.5	Genetic Toxicity *In Vitro*			
A.	Bacterial Test:	S. typhimurium TA98, TA100, TA1535, TA1537 and TA1538	Ames Test; Neodene 8	Negative - (with and without activation)
		S. typhimurium, TA98, TA100, TA1535, TA1537 and TA1538 and E. coli mutant WP2 uvrA	Ames Test; 1-octene	Negative - (with and without activation)
B.	Non-Bacterial Test:	Chinese Hamster Ovary Cells	Chromosomal Abberration Assay;	Negative- with and without activation
		Chinese Hamster Ovary Cells	Chromosomal Abberration Assay;	Questionable results with activation; aberration rate increased approx. 2-fold over background, but no dose response; negative without activation.
		Balb/c-3T3	Cell Transformation	Negative with and without activation
5.6	Genetic Toxicity *In Vivo*	-----	-----	N/D
5.8	Toxicity to Reproduction	-----	-----	N/D
5.9	Developmental Toxicity/Teratogenicity	-----	-----	N/D
5.10	Other:	Rat	Used C_{6-8} alkenes	Aspiration Hazard
5.11	Experience with Human Exposure	-----	-----	N/D

N/A = not applicable N/D = not determined AO = alpha olefin

Unless noted, all test substances are considered to contain >90% 1-octene. This would include those tests that were conducted using Neodene 8 and Alpha Olefin 8. Special blends will be described appropriately.

*****C_{6-8} AO blend consists of: $<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%

SIDS DOSSIER
(1-OCTENE: CAS No 111-66-0)

SIDS SUMMARY

CAS NO: 111-66-0 1-octene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
PHYSICAL-CHEMICAL								
2.1	Melting Point	Y	N	N	N	N	Y	N
2.2	Boiling Point	Y	N	N	N	N	Y	N
2.3	Vapour Pressure	Y	N	N	Y	Y	Y	N
2.4	Partition Coefficient	Y	N	N	Y	?	Y	N
2.5	Water Solubility	Y	N	N	Y	N	Y	N
OTHER STUDIES RECEVED								
2.6	Flash Point	Y	N	N	Y	N	Y	N
2.7	Flammability	N	N	N	N	N	Y	N
2.9	Density	Y	N	N	N	N	Y	N
ENVIRONMENTAL FATE/ BIODEGRADATION								
3.5	Aerobic Biodegradability	Y	Y	N	Y	N		N
3.5	Abiotic Degradability	N						N
3.1.2	Hydrolysis	Y	N	N	N	Y	Y	N
3.1.1	Photodegradability	Y	N	N	N	Y	Y	N
3.3	Env. Fate/Distribution	Y	N	N	N	Y	Y	N
	Env. Concentration	N						
OTHER STUDIES RECEIVED ECOTOXICOLOGY								
4.1	Acute Toxicity Fish	Y	Y	N	Y	N	Y	N
4.2	Acute Toxicity Daphnia	Y	Y	N	Y	N	Y	N
4.3	Toxicity to Algae	Y	Y	N	N	Y	Y	N
4.4	Toxicity to Bacteria	Y	Y	N	N	N	Y	N
4.5.2	Chronic Toxicity to							
	- Daphnia	Y	N	N	N	Y	Y	N
	- Algae	Y	N	N	N	Y	Y	N
	- Fish	Y	N	N	N	Y	Y	N
4.6.1	- Terrest. Organisms	N						
4.6.2	- Terrest. Plants	N						
4.6.3	- Avians	N						
4.6.4	Avian Reproduction	N						
OTHER STUDIES RECEIVED TOXICOLOGY								
5.1.1	Acute Oral	Y	Y	N	Y	N	Y	N
5.1.2	Acute Inhalation	Y	N	N	Y	N	Y	N
5.1.3	Acute Dermal	Y	Y	N	Y	N	Y	N
5.2.1	Corrosivity, Irritation	Y	Y	N	Y	N	Y	N
5.2.2	Eye Irritation	Y	Y	N	Y	N	Y	N
5.3	Skin Sensitization	Y	Y	N	Y	N	Y	N
5.4	Repeated Dose	Y	Y	N	Y	N	Y	N

CAS NO: 11-66-0 Octene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
5.5	Genetic Toxicity							
	- Gene Mutation	Y	Y	N	Y	N	Y	N
	- Chromosomal Aberrations	Y	Y	N	Y	N	Y	N
5.8	Reproductive Toxicity	N	N	N	N	N	Y	N
5.12	Metabolism	N	N	N	N	N	Y	N
OTHER STUDIES RECEIVED								

SIDS PROFILE

1.1	CAS NO.	111-66-0
1.2	CHEMICAL NAME	1-OCTENE
1.5	STRUCTURAL FORMULA	C_8H_{16}
	OTHER CHEMICAL INFORMATION	SYNONYM: OCTENE-1; Alpha Olefin 8, NERATEN®8
3.0	SOURCES AND LEVELS OF EXPOSURE	MANUF./PRODUCTION AND PROCESSING ACTIVITIES
3.1	PRODUCTION RANGE	34,580 metric tonnes
3.3	CATEGORIES AND TYPES OF USE	USED AS A CO-MONOMER IN CERTAIN OLEFIN PRODUCTS; USED IN THE PRODUCTION OF PLASTICIZERS; OTHER INDUSTRIAL USES
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)		

Summary of Responses to the OECD Request for Available Data on HPV Chemicals

REVISED: October 1999

1. General Information

1.01 Substance Information:

A. CAS number: 111-66-0

B. Name (IUPAC): 1-Octene

C. Name (OECD):

D. CAS Descriptor:

E. EINECS-Number:

F. Molecular Formula: C_8H_{16}

G. Structural Formula: $CH_3 - (CH_2)_5 - CH = CH_2$

H. Substance Group: Alkene

I. Substance Remark:

J. Molecular Weight: 112.1

1.02 OECD Information

A. Sponsor Country: United States

B. Lead Organization: United States Environmental Protection Agency

Contact Point:
Mr. Oscar Hernandez
US Environmental Protection Agency (USEPA)
Director Risk Assessment Division (USEPA/OPPTS/RAD/7403)
401 M Street S.W.
Washington, DC 20460
TELEPHONE: 1-202-260-1832
TELEFAX : 1-202-260-1216

C. Name of Responder:

American Chemistry Council (Higher Olefins Panel)
1300 Wilson Blvd.
Alexandria, Virginia 22209, USA

Panel Manager: Doug Anderson
Telephone: (703) 741-5616
Fax: (703) 741-6091

1.1 General Substance Information

A. Type of Substance: Organic

B. Physical State: Liquid

C. Purity of Industrial product: Varies but usually 99.1%

1.2 Synonyms: Octene-1; 1-Octene

1.3 Impurities: C_6 and lighter = 0.1 wt.%;
C_{10} and higher = 0.8 wt.%;
CAS no. 1632-16-2, 2-ethylhex-1-ene < 2.2% w/w

1.4 Additives: None

1.5 Quantity: U.S.A. – 1986, 1990, 1994 and 1998 production volume aggregate figures range from 100 – 500 million pounds. (Reference: US EPA, CUS Report (10/99) non – CBI TSCA inventory)

1.6 Labeling and Classification:

International transport classification	
UN Number	1993
Class	3.2
Packaging group	2
Hazard identity no.	33
Proper shipping name	Flammable liquids, N.O.S. (1-octene)
CEFIC-Tremcard no.	30G30
ADR and RID (road, railway)	
Class	3, 3b.
Symbol	Flammable liquid
Proper shipping name:	1-octene, 3, 3b, ADR
IATA/ICAO (air)	
Class	3
Packing group	3
Symbol	Flammable liquid
Proper shipping name:	Flammable liquids, N.O.S. (1-octene)
IMO/IMDG (sea)	
Class	3.2
Page	3230
EmS-No	3-07
MFAG-No	310
Packing group	III
Symbol	Flammable liquids, N.O.S. (1-octene)

EEC-labelling (recommendation)

R-phrases	11 Highly flammable—11-36/37/38-65 (Spolane recommendations)
S-phrases	9-16-29-33 Keep container in a well-ventilated place. Keep away from sources of ignition--No smoking Do not empty into drains—Take precautionary measures against static discharges. S16-24/25-26-46-62 (Spolane recommendations)

1.7 Use Pattern:

A. General Use Pattern:

Industrial Uses: - in closed systems.

Use categories: (1) Co-monomer in certain olefin products; (2) Production of plasticizers; (3) Others

1.8 Occupational Exposure Limit Value: Not established

1.9 Sources of Exposure:

1.9.1 Manufacturing and Processing:

No data available on workplace concentrations for Ethyl or users. Occupational and environmental exposure expected to be low due to handling in closed systems. Potential occupational exposure occurs via inhalation of vapors (low ppm range). Calculated estimations of emissions are: (1) Air ≈ 23 tons/year; (2) Water < 1 ton/year; and (3) Organic Waste ≈ 1 ton/year.

Reference: d) Ethyl Corporation

1.10 Additional Remarks: Waste Disposal: United States – regulated as hazardous waste must be disposed of in a "permitted" hazardous waste facility in compliance with EPA and/or other applicable local, state and federal regulations. Reportable Quantity = 100 pounds for ignitable substances.

DOT Descriptor/Proper Shipping: Petroleum Naptha
DOT Hazard Class: Flammable liquid
DOT ID: UN1255

2. Physical-Chemical Data

2.1 Melting or Decomposition Point: -101.73° Centigrade
Method (e.g., OECD, others): Not specified.
GLP: YES [ ]
NO [N]

Reference: a) Handbook of Chemistry and Physics (1975)

2.2 Boiling Point: Range: 5% ... 121°C at 1 atm.;
95% ...123°C at 1 atm.

Method (e.g., OECD, others): Not mentioned
GLP: YES [ ]
NO [N]

Reference: b) Alpha Olefins Applications Handbook

2.3 Density:

0.7149[a] g/ml @ 20 deg C
0.715[b] g/ml @ 20 deg C

Reference: (a) Handbook of Chemistry and Physics
(b) Alpha Olefins Applications Handbook

2.4 Vapor Pressure

(15.2 mm Hg) (.1333) = 2.03 kPa at 20°C (measured) (20.3 hPa)
(17.4 mm Hg) (.1333) = 2.32 kPa at 25°C (calculated) (23.2 hPa)

Method (e.g., OECD, others): Not specified.
GLP: YES [ ]
NO [N]

Reference: b) Alpha Olefins Application Handbook

2.5A. Partition coefficient n-Octanol/water

log P_{ow} = 4.4 – 5.5 at pH 6.7

Method: calculated [X]
measured [ ]

GLP: YES [ ]
NO [N]

Analytical Method: C 6 – C8 AO Blend

Reference: ?

B. Partition coefficient n-Octanol/water

Log Pow = 3.5 – 4.6

Method: calculated [ ]
Measured [X]

GLP: no data

Analytical Method: C6 – C8 AO Blend

Reference: ?

C. Partition coefficient n-Octanol/water

Log Pow = 4.57 @ 25^0C

Method: calculated [ ]
Measured [X]
GLP: no data

Reference: Y.B. Tewari, M.M. Miller, S.P. Wasik & D.E. Martine, J. Chem. Eng. Data 27 (1982), 451 - 454

2.6A Water solubility

A. 4.1 mg/l at 25°C

Method (e.g., OECD, others):
GLP: YES [ ]
NO [X]

Analytical Method:

Comments: Description of very low solubility

Reference: Y.B. Tewari, M.M. Miller, S.P. Wasik & D.E. Martine, J. Chem. Eng. Data 27 (1982), 451 - 454

B. Results: Negligible
Method (e.g., OECD, others):
GLP: YES [ ]
NO [X]

Analytical Method:

Reference: Ethyl Corporation, Material Safety Data Sheet (MSDS)

2.6B pH/pKa – Not available

2.7 Flash point (liquids)

A. 10°C closed cup [X] open cup [ ]

Method (e.g., OECD, others including reference to the standard test used):
GLP: YES [ ]
NO [N]
Comments:
Reference: b) Alpha Olefins Applications Handbook

B. 21^0C closed cup [ ] open cup [ ]

Method (e.g., OECD, others including reference to the standard test used):
GLP: YES [ ]
NO [N]
Comments:
Reference: Aldrich Catalog and Merck Index, 11^{th} edition.

2.8 Auto Flammability: No data available

2.9 Flammability: No data available

2.10 Explosive Properties:

Lower Explosive Limit (LEL) = 0.8%
Upper Explosive Limit (UEL) = 6.7%

Reference: Ethyl Corporation, Material Safety Data Sheet (MSDS)

2.11 Oxidizing Properties: No data available

2.12 Oxidation: Reduction Potential: No data available

2.13 Additional Remarks:

2.13A Viscosity 0.492[b] cP/20 deg C and 0.313[b]/50 deg

2.13B Solubility[c]-Practically insol. in H_2O;Miscible with ethanol, ether.
Solubility[a]-Sol. in acetone, benzene, chloroform; very soluble in organic solvents.

Comments:

Reference: (a) Handbook of Chemistry and Physics
(b) Alpha Olefins Applications Handbook
(c) The Merck Index

2.13C Vapor Density: 3.9 (air = 1)
Reference: Ethyl Corporation, Material Safety Data Sheet (MSDS)

2.13D Specific Gravity: 0.72
Reference: Ethyl Corporation, Material Safety Data Sheet (MSDS)

2.13E Evaporation Rate: 1.3 (butyl acetate = 1)
Reference: Ethyl Corporation, Material Safety Data Sheet, (MSDS)

3. Environmental Fate and Pathways:

3.1 Stability:

3.1.1.a. Photodegradation: Stability in air (e.g., photodegradability) and in water (e.g. hydrolysis)
Test Substance: >97% Octene
Test Method or estimation method: measured but not described in detail
GLP Yes [ ]
No [X]
Test Results: Sensitizer: OH
Concentration of sensitizer: 1,000,000 molecule/cm3
Rate of Constant: 0000000000409 cm3/molecule*sec
Degradation: 50% after 4.71 hour

Reference: R. Atkinson, Chem. Rev. 85 (1985), 69 –201

3.1.1.b. Photodegradation:
Test Substance: 1-Octene
Test Method or estimation method: Estimated utilizing the US EPA's EPIWIN computer model.
GLP Yes [ ]
No [X]
Test Results: half-life with ozone = approximately 22 hours
Half-life with hydroxy radical = approximately 3.8 hours

Reference: US EPA, EPIWIN output run by Amuel Kennedy dated 9/99.

3.1.2. Stability in Water: Hydrolysis: No data

3.1.3. Stability in Soil:

A. Soil Adsorption
Test Substance: ($C_6 - C_{12}$) Alpha Olefins
Test Method or estimation method: Estimated
GLP Yes [ ]
No [X]

Test Results: The C6 –C12 alkenes are expected to volatize from the soil surface to the atmosphere. The high soil adsorption coefficients determined for these compounds range from 3,500 to 660,000 suggesting that they will be essentially immobile in soil except when large volumes of material are present to aid in the dissolution of the alkenes (i.e. leaking underground storage tank (gasoline)). Thus, they are not expected to leach into ground water. Strong adsorption to soil may attentuate the rate at which they volatize to the atmosphere.

Reference: ITC, IR-427 Update (1990-1991)

B. Soil Adsorption

Test Substance: 1-Octene

Test Method or estimation method: Estimated utilizing the US EPA's EPIWIN computer model

GLP Yes [ ]
No [X]

Test Results: Indicate that based on a vapour pressure of 17.4 and a Koc value of 507, that soil mobility was predicted to be moderate. 1-octene was predicted to possibly be present in dry soil and that it if present in moist soil mobility would be rapid. Eventhough 1-octene may exist in dry soil it is

believed that since the vapour pressure is greater than 1 mmHg that volatilization will occur prior to mobility being an issue.

Reference: US EPA EPIWIN output run by US EPA/OPPT/RAD/ECAB Amuel Kennedy, 9/99.
EAB-IRER, 1997.

3.2 Monitoring Data: (Environment)

Calculated estimations of emissions are: (1) Air ≈ 23 tons/year; (2) Water < 1 ton/year; and (3) Organic Waste ≈ 1 ton/year.

Reference: d) Ethyl Corporation

3.3. Transport and Distribution between environmental compartments including estimated environmental concentrations and distribution pathways.

3.3.1 Transport: Volatilization from Water:
Test Substance: 1-Octene
Test Method or estimation method: Estimated utilizing the US EPA's EPIWIN computer model
GLP Yes [ ]
No [X]

Test Results: half-life from a model river = 1 hour, half-life from a model lake = 4 days. The chemical is not expected to persist in a river or lake within a significant amount of time.

Reference: US EPA, EPIWIN output run by Amuel Kennedy dated 9/99.

3.3.2.1 Theoretical Distribution (Fugacity Calculations)

A. Type of transport and distribution processes between compartments

Media: air-biota-sediment(s) – soil- water
Estimation of environmental concentrations:
Results of the estimation:

Level III Utilizing default emission values: Air: 5.52%; Water: 56.3%; Soil: 34.1%; Sediment: 4.08%

Level III Utilizing estimated emission values as provided by American Chemistry Council (10 kg/hr to air, 1 kg/hr to water, 0 kg/hr to soil)

Air: 15%, Water: 61%; Soil: <1%; Sediment: 23%.

Summary of the method (or model) used: Calculation method –EQC model—Mackay Fugacity level III

Reference: USEPA/OPPT/EETD/EAB; EQC model output for 1-octene. David Lynch, (11/17/2000)

B. Type of transport and distribution processes between compartments

Media: air-biota-sediment(s) – soil- water
Estimation of environmental concentrations:
Results of the estimation: Air: 100%; Water: <1%; Soil: <1%; Sediment: <1%
Summary of the method (or model) used: Calculation method –EQC model—Mackay Fugacity level I

Reference: EQC model output for 1-octene. USEPA/OPPT/EETD/EAB; David Lynch, (11/17/2000) and D. Mackay, Multimedia Environmental Models: The fugacity approach. Lewis Publishers Inc. Chelsea Michigan USA, 1991, Chptr 5.

3.4 Mode of Degradation in Actual Use:

3.5. Biodegradation

A.
Test Substance: 1-Octene
Test Type: aerobic [X], anaerobic [ ]
Test Medium: Water
Inoculum: Psuedomonas fluorescens

Test Results: Degradation: 41 – 42% after 28 day—inherently biodegradable

Reference: Adema, D.M.M. and G.H. Bakker (1985)

B.
Test Substance: Olefin 68 PQ11 (C_6-C_8 Cracked Wax Olefin)
$<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%

Test Type: aerobic [X], anaerobic [ ]
Test Medium:
Inoculum: Psuedomonas fluroescens
Test Method: OECD guideline 301D
GLP: YES [X]
NO [ ]

Test Results: Degradation: 2—4% after 41 day—very slowly biodegradable

Reference: Adema, D.M.M. and G.H. Bakker (1985).

C.
Test Substance: 1-Octene
Test Type: aerobic [X], anaerobic [ ]
Test Method: Predicted using US EPA EPIWIN

Test Results: Rate of biodegradation, days to weeks—volatilization is expected to be more rapid than biodegradation.

Reference: US EPA EPWIN output run by US EPA OPPT/RAD/ECAB Amuel Kennedy, 9/99.

3.6 BOD-5, COD or Ratio BOD-5/COD: No data available

3.7 Bioaccumulation: No data available

3.8 Additional Remarks:

A. Sewage Treatment:

Test Substance: 1-Octene
Test Type: aerobic [X], anaerobic [ ]
Test Medium: secondary wastewater treatment (water)
Inoculum:
Test Method: Calculated, EPIWIN, secondary wastewater treatment removal model
GLP: YES [ ]
NO [X]

	Test Results:	>99% removed from secondary wastewater treatment.
	Comments:	Extensive stripping to air is predicted and biodegradation potential is high
	Reference:	EAB-IRER (1995), model run by US EPA/OPPT/EAB
B.	Other:	Migration in Ground Water
	Rate:	Moderate
	Comments:	may be mitigated by volatilization
	Reference:	EAB-IRER (1997) US EPA EPIWIN output run by US EPA/OPPT/RAD/ECAB Amuel Kennedy, 9/99.

4. Ecotoxicological Data

4.1. Acute/prolonged toxicity to Fish

A.
Results of acute tests: LC50 (96 hr) = 100 mg/l
Test substance: Olefins 68 PQ11 (C_6-C_8 Cracked Wax Olefin Mixture)
$<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%
Test species: Salmo gairdneri
Test method (e.g., OECD, others): ??
Type of test: static [X], semi-static [ ], flow-through [ ]
Other (e.g., field observation) [ ]

GLP: YES [X]
NO [ ]

Test results: LC50 (96hr) = 100 mg/l
Comments:

Reference: Shell Research Limited Group Research Report: SBGR.83. 357

B.
Results of acute tests: NOEC (96 hr) = 3.2 mg/l; LC50 (96 hr) = 4.8
Test substance: 1-Octene
Test species: Brachydanio rerio

Test method (e.g., OECD, others): Test solutions were prepared by adding test substance to 1 liter of fresh water and stirring for 4 hours in glass-stoppered flasks before adding the test animals. Ten animals/dose level were tested in a glass beaker covered with a watch glass. The test compound was not visible during the test period.
Concentration tested: 0, 3.2, 10 and 32 mg/l.

Type of test: static [X], semi-static [], flow-through [ ]
Other (e.g., field observation) [ ]
GLP: YES [ ]
NO [X]
Test results: LC_{50} (24 hr) = 10 mg/l
LC_{50} (48 hr) = 4.8 mg/l
LC_{50} (72 hr) = 4.8 mg/l
LC_{50} (96 hr) = 4.8 mg/l

NOEC (96 hr) = 3.2 mg/l;

Comments: Condition of test animals compared to the controls was by visual estimation

Reference: Adema, D.M.M. and G.H. Bakker (1985)

C.
Results of acute tests: NOEC (96hr) = 3.2 mg/l;
Test substance: 1-Octene
Test species: Brachydanio rerio

Test method (e.g., OECD, others): Test solutions were prepared by adding test substance to 1 liter of fresh water and stirring for 4 hours in glass-stoppered flasks before adding the test animals. Ten animals/dose level were tested in a glass-stoppered beaker. The test compound was not visible during the test period. Concentration tested: 0, 3.2, 10 and 32 mg/l.

Type of test: static [X], semi-static [ ], flow-through [ ]
Other (e.g., field observation) [ ]

GLP: YES [ ]
NO [ ]
Test results: LC_{50} (24 hr) = >3.2 <10
LC_{50} (48 hr) = >3.2 <10

LC_{50} (72 hr) = >3.2 <10
LC_{50} (96 hr) = >3.2 <10 estimated to be about 6

NOEC (96 hr) = 3.2 mg/l

Comments: Condition of test animals compared to the controls by visual estimation

Reference: Adema, D.M.M. and G.H. Bakker (1985)

D. Test Substance: 1-Octene
Test Method: Predicted by EPA ECOSAR model (input) Log Kow = 4.57, Water solubility = 4.1 mg/l, MW = 112.22.

Test Results: Test Species: Fish (fresh water)
LC50 (96hr) = 0.319 ppm

Test Species: Fish (saltwater)
LC50 (96hr) = 0.253 ppm

Reference: USEPA ECOSAR model output for 1-octene.
USEPA/OPPT/RAD/ECAB, Amuel Kennedy (8/20/99)

4.2 Acute Toxicity to Aquatic Invertebrates - daphnids

A. Test substance: 1-Octene
Test species: Daphnia Magna

Test method (e.g., OECD, others): Test solutions were prepared by adding test substance to fresh water and stirring for 4 hours in glass-stoppered flasks. 25 animals were exposed to the test substance in 500 ml of test solutions in a glass beaker, covered with a watch glass. Another assay was conducted in which a glass-stoppered flask was used as the testing vessel. Test compound was not visible during the test period.
GLP: YES [ ]
NO [X]

Test results: Beaker covered with watch glass:
EC50 (48hr) = >3.2 <10 mg/l (estimated to be about 7);
NOEC (48hr) = 3.2 mg/l

Stoppered flask:
EC_{50} (48 hr) = >3.2<10 mg/l (estimated to be about 6);
NOEC (48 hr) = 3.2 mg/l

Comments: Condition of test animals compared to the controls (visual estimation)

Reference: Adema, D.M.M. and G.H. Bakker (1985)

B. Test substance: Olefins 68 PQ 11 (C_6- C_8 Cracked Wax Olefins Mixture)
$<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%
Test species: Daphnia Magna
Test method (e.g., OECD, others): other
GLP: YES [ ]
NO [X]
Test results: EC50 (48hr) = 67 mg/l
Comments:
Reference: Shell Research Limited Group Research Report SBGR.83.357.

C. Test Substance: 1-Octene
Test Method: Predicted by EPA EPIWIN/ECOSAR model (input) Log Kow = 4.57,
Water solubility = 4.1 mg/l, MW = 112.22.

Test Species: Daphnia
Test Results: LC50 (48hr) = 0.409 ppm
Reference: USEPA EPIWIN/ECOSAR model output for 1-octene. USEPA/OPPT/RAD/ECAB, Amuel Kennedy (8/20/99)

4.3 Toxicity to Aquatic Plants, e.g. algae

A. Test substance: Olefins 68 PQ 11 (C_6-C_8 Cracked Wax Olefins Mixture) $<C_6$ = 0.4%, C_6 = 47.8%, C_7 = 36.2%, C_8 = 15.8%, $>C_8$ = 0.1%
Test species: Selenastrum capricornutum
Test method (e.g., OECD, others): 4-day Growth Method
GLP: YES [X] NO [ ]
Test results: EC50 (96hr) = 200 mg/l
Comments:
Reference: Shell Research Limited Group Research Report SBGR. 83.357.

B. Test Substance: 1-Octene
Test Method: Predicted by EPA ECOSAR model (input) Log Kow = 4.57, Water solubility = 4.1 mg/l, MW = 112.22.

Test Results:
Acute:
Test Species: Green Algae
EC50 (96hr) = 0.296 ppm

Chronic:
Test Species: Green Algae
ChV (96hr) = 0.131 ppm

Reference: USEPA ECOSAR model output for 1-octene. USEPA/OPPT/RAD/ECAB, Amuel Kennedy (8/20/99)

4.4 Toxicity to Bacteria

Test substance:
Test species: Pseudomonas fluorescens
Test method (e.g., OECD, others): other
Type of test: static [ ], semi-static [ ], flow-through [ ]
Other (e.g., field observation) [ ]

GLP: YES [ ] NO [X]
Test results: IC50 = 370 mg/l
Comments: Microbial Inhibition Test
Reference:

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
Test Substance: 1-Octene
Test Method: Predicted by EPA ECOSAR model (input) Log Kow = 4.57, Water solubility = 4.1 mg/l, MW = 112.22.
Test Results: Test Species: Fish (fresh water)
LC50 (14day) = 0.870 ppm, ChV (30 day) = 0.062 ppm

Reference: USEPA ECOSAR model output for 1-octene. USEPA/OPPT/RAD/ECAB, Amuel Kennedy (8/20/99)

4.5.2 Chronic Toxicity to Aquatic Invertebrates (Daphnia Reproduction)
Test Substance: 1-Octene

Test Method:	Predicted by EPA ECOSAR model (input) Log Kow = 4.57, Water solubility = 4.1 mg/l, MW = 112.22.
Test Results:	Test Species: Daphnia EC50 (16 day) = 0.065 ppm
	Test Species: Green Algae ChV (96hr) = 0.131 ppm
Reference:	USEPA ECOSAR model output for 1-octene. USEPA/OPPT/RAD/ECAB, Amuel Kennedy (8/20/99)

4.6 Toxicity to terrestrial organisms: No data available

4.6.1 Toxicity to soil dwelling organisms: No data available
4.6.2 Toxicity to terrestrial plants: No data available
4.6.3 Toxicity to other Non-Mammalian Terrestrial Species (birds): No data available

4.7 Biological Effects Monitoring: No data available

4.8 Biotransformation and Kinetics: No data available

4.9 Additional Remarks:

5. Toxicity

5.1. Acute Toxicity

5.1.1. Acute oral toxicity

A. Test substance: 1-Octene (Ethyl Corporation)
Test species/strain: Sprague-Dawley rats, males
Test method (e.g., OECD, limit test, fixed dose test):
GLP: YES [ ]
NO [X]

Test results: LD50 > 10 g/kg.
Discriminating dose (for fixed dose only):
Comments: Ten male rats were given single dose of 10 grams/kg.

Reference: e) Ethyl Corporation, 1973

B. Test substance: NEODENE-8 Alpha Olefin
Test species/strain: Fischer 344 rats, 5 males, 5 females in confirmation group.
Test method (e.g., OECD, limit test, fixed dose test):
GLP: YES [X] 21 CFR Part 58
NO [ ]
Test results: LD50 > 5 ml/kg ; >5000mg/kg
Discriminating dose (for fixed dose only):

Comments: Undiluted NEODENE 8 Alpha Olefin caused no deaths at volumes of 1.0, 2.5, and 5 ml/kg body weight. The confirmation dose of 5.0 ml/kg given to 10 animals (5 female, 5 male) caused no deaths.

Reference: f) Shell Development Company; Acute Oral Toxicity of Neodene 8 Alpha Olefin in the Rat, WRC-RIR 286.

5.1.2 Acute inhalation toxicity

Test substance: 1-Octene (Ethyl Corporation)
Test species/strain: Sprague-Dawley rats, male
Test method (e.g., OECD, EC limit test): other
GLP: YES [ ]
NO [X]

Test results: LC50 (4hr): 8,050 ppm (95% C.L. 6,600-9,800 ppm)

Comments: Six groups of 10 male rats each were exposed to concentrations ranging from 6,050 to 11,580 ppm for 4 hours. All deaths occurred within the exposure. A preliminary one hour study at the saturated vapor limit (87.5 mg/l nominal concentration; 19,110 ppm) caused deaths in 9 of 10 male Sprague Dawley rats. Necrospy revealed hemorrhagic lungs, very pale kidneys and nutmeg livers. The one surviving animal was observed 14 days after exposure, sacrificed and autopsied—There were no signs of gross pathological changes 14 days after exposure.

Reference: e) Ethyl Corporation

5.1.3. Acute dermal toxicity

A. Test substance: 1-Octene (Ethyl Corporation)
Test species/strain: New Zealand White Rabbits
Test method (e.g., OECD, limit test):
GLP: YES [ ]
NO [X]

Test results: Dermal LD50 > 10 g/kg; 10,000 mg/kg

Comments: Four rabbits were used (two with abraded sites) had undiluted 1-octene applied at a dose of 10 g/kg/ bw for 24 hrs. There were no deaths.

Reference: e) Ethyl Corporation

B. Test substance: NEODENE-8 Alpha Olefin
Test species/strain: New Zealand White Rabbits
Test method (e.g., OECD, limit test):
GLP: YES [X] 21 CFR Part 58
NO [ ]

Test results: Dermal LD50 1.43 g/kg

Comments: Groups of 16 (8 M, 8 F) rabbits were dosed with 2 ml/kg undiluted test material (NEODOL-8) under an occlusive dressing for 24 hours. There were no deaths or major gross pathological changes. Mild to moderate skin irritation was present at the site of application, after patch removal, which became less pronounced (but not fully reversed) over 14 days.
Original study indicated a Dermal LD_{50} >2 ml/kg/bw however US EPA review indicates that the LD_{50} should be changed to reflect 1.43 g/kg in a memo date 8/14/96. As a result the LD_{50} for this study was changed from > 2 ml/kg/bw to 1.43 g/kg.

Reference: g) Shell Development Company, Report WRC RIR-288,

5.2 Corrosiveness/Irritation

5.2.1 Skin irritation

A. Test substance: 1-Octene (Ethyl Corporation)
Test species/strain: New Zealand White Rabbits (six)
Test method (e.g., OECD, others): FHSA method, Draize scoring, 24 hour contact.
GLP: YES [ ]
NO [X]

Test results: Draize score 1.8 out of a possible total of 8.0. Mean erythema scores 2.0 at 72 hours. Slightly irritating but classified as not irritating.

Comments: Erythema was 83% of the Draize score; edema was 17%.

Reference: e) Ethyl Corporation

B. Test substance: NEODENE 8 Alpha Olefin
Test species/strain: New Zealand White Rabbits (six)
Test method (e.g., OECD, others): FHSA method, Draize scoring was made at 24 and 72 hour contact for erythema and oedema. Intact and abraded sites. (further scoring was conducted at 7days)
GLP: YES [X] 21 CFR Part 58
NO [ ]

Test results: Primary Irritation Index score 3.38 (max. 8.0), the material was moderately irritating, although this time period does not fully reflect the nature of the reaction. Classified as irritating
Comments: Further scoring at 7 days showed eschar formation and severe edema)

Reference: h) Shell Development Company, Report WRC RIR-283, 1983

C. Test substance: Gulftene 8 Alpha Olefin

Test species/strain: New Zealand White Rabbits
Test method (e.g., OECD, others): OECD Guideline 404. One-half ml undiluted material was applied to 6 rabbits, with unabraded skin under a semi-occluded dressing. Scores were made for erythema and edema at 1, 24, 48 and 72 hr, and at 7 and 14 days after initiation of exposure.

GLP: YES [X]
NO [ ]

Test results: The 4-hr exposure produced well-defined erythema and slight to severe edema which cleared by day 7. Other dermal reactions noted were desquamation and crust formation which persisted to day 14, but were considered to be reversible effects. The Draize primary irritation index was 3.42. The mean 24-72 scores for erythema and edema were1.9 and 1.1 respectively. Classified as not irritating

Comments:

Reference: Driscoll, R., Chevron Chemical Company, sponsor, Acute dermal irritation test in the rabbit with Gulftene 8, Safepharm Laboratories Ltd. Report 703/076, 1996.

D. Test substance: 1-Octene (Ethyl Corporation)
Test species/strain: New Zealand White rabbits
Test method (e.g., OECD, others): 28 Day Repeated Dose Skin Irritation
GLP: YES [ ]
NO [X]

Test results:Treated animals had questionable hyperemia, questionable exfoliation, and questionable scab formation at the end of the study.

Comments: Dosing was 0.2 ml to the test sites of 6 animals for 5 days per week for 20 applications over a 28-day period. Scoring was done 24 hours after each application. Study was limited to one dose level and macroscopic observations.

Reference: e) Ethyl Corporation

5.2.2 Eye Irritation

A. Test substance: 1-Octene (Ethyl Corporation)
Test species/strain: New Zealand White Rabbits
Test method (e.g., OECD, others): FHSA method, 0.1 ml volume, no wash out, Draize scoring at 24, 48, and 72 hours.
GLP: YES [ ]
NO [X]

Test results: All scores zero, except one conjunctival score of 2 at 24 hours. Result not irritating and classified as not irritating.
Comments:

Reference: e) Ethyl Corporation

B. Test substance: NEODENE 8 Alpha Olefin
Test species/strain: New Zealand White Rabbits
Test method (e.g., OECD, others): FHSA method, 9 rabbits, 0.1 ml volume, with washout and without, Draize scoring at 1, 24, 48, and 72 hours and 7 days.

GLP: YES [X] 21 CFR Part 58

NO [ ]

Test results:Mean Draize score was 4.7 (out of 110) at 1 hour after exposure for the washed eye animals and 0.0 at other points. Nonwashed scores were 3.0 at one hour, 0.3 at 24 hours and 0.0 thereafter. Results were slightly irritating; classified as non-irritating.

Comments:

Reference: i) Shell Development Company

5.3 Skin sensitization

Test substance: NEODENE 8 Alpha Olefin
Test species/strain: Duncan Hartley albino guinea pigs (5 male/5 female)
Test method (e.g., OECD, others): Beuhler method; Test articles: 1% w/v NEODENE-8 Alpha Olefin in absolute ethanol, absolute ethanol (vehicle control), or 2,4 dinitrochlorobenzene as 0.1% w/v solution (positive control). Administered 1 day/week, 6 hr/day for 3 weeks.
GLP: YES [X] 21 CFR Part 58
NO [ ]

Test results: Negative; Not sensitizing

Comments: No increase in irritation over the 5 week test period. At challenge, one test animal compared to 2 vehicle control animals had scores of +/- to 0 at 48 hours.

Reference: j) Shell Development Company, Report WRC RIR-285, 1983

5.4 Repeated dose toxicity

Oral Repeated dose toxicity
Test substance: 1-Octene (Netherlands)
Test species/strain: Rats: Strain Unknown
Test method (e.g., OECD, others):Sub-chronic (90 day) Gavage
GLP: YES [ ]
NO [X]

Test results: No-toxic-effect level is between 50 and 500 mg/kg b.w./day, and probably only slightly less than 500 mg/kg/b.w./day. (see comments)

Groups of 40 (20M, 20F) rats were gavaged with 0, 5,50 or 500 mg/kg body weight/day for 7 days a week for 13 weeks. Body weights, food intake, clincial signs, behavior, and hematological parameters did not differ significantly. Gross necropsy findings were not different. Slight changes differing from control were only seen in the high dose group, and included increased kidney weights and decreased plasma chloride in both sexes, increased urinary volume and unspecified microscopic kidney differences in male rats only, and increased plasma creatinine in females only.

Comments: Based on data presented, the only NOEL that was determined is 50 mg/kg/day. This is due to the limitations of doses utilized in the study design and treatment related effects observed at 500 mg/kg/day.

Reference: n) DSM, Beek, the Netherlands (Report No. V86.408/251091

5.5 Genetic toxicity

A. Bacterial test (gene mutation assay)

1. Test substance: NEODENE 8 Alpha Olefin
Test species/strain: Salmonella Typhimurium Strains TA98, TA100, TA1535, TA1537, and TA1538
Test method (e.g., OECD, others): Ames test, with and without metabolic activation from rat liver homogenate fraction, modification by preincubation plate incorporation
GLP: YES [X] 21 CFR 58
NO [ ]

Test results: Negative. No indication of mutagenic response in any of the five Salmonella typhimurium strain in presence or absence of metabolic activation fraction. Concentrations tested ranged from 0.45 mg/plate (toxic) to 1.4x10-4 mg/plate.

Concentration of the test compound resulting in precipitation: 14 ug/plate to 0.45 mg/plate (toxic)

Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[X]
without metabolic activation:	[ ]	[ ]	[X]

Comments: Solvents were absolute ethyl alcohol (test article) and DMSO (positive control). Positive controls were 2-aminoanthracene, 2-Nitrofluorene, N-Methyl-N'-nitro-N-nitrosoguanidine, and 9-Aminoacridine hydrochloride monohydrate.

Reference: k) Shell Development Company, WRC, RIR-28

2. Test substance: 1-Octene (Netherlands)
Test species/strain: Salmonella Typhimurium Strains TA98, TA100, TA1535, TA1537, and TA1538, and Escherichia coli mutant WP2 uvrA
Test method (e.g., OECD, others): Ames test, with and without metabolic activation from rat liver homogenate fraction S-9 mix
GLP: YES [ ]
NO [X]
Test results: No indication of mutagenic response in any bacterial strain in presence or absence of metabolic activation fraction.

Concentration of the test compound resulting in precipitation:
Genotoxic effects:

	+	?	-
with metabolic activation:	[ ]	[ ]	[x]
without metabolic activation:	[ ]	[ ]	[x]

Comments: Details not known

Reference: o) DSM, Geleen, the Netherlands, Report No. 85.528/250064

B. Non-bacterial in vitro test

1. (cell transformation)

Test substance: NEODENE 8 Alpha Olefin

Type of cell used: Balb/c-3T3 cell system
Test method (e.g., OECD, others): Morphologic transformation assay of Balb/c 3T3 cells
GLP: YES [X]
NO [ ]

Test results: Test material was considered to be inactive as a Balb/c-3T3 transforming agent the absence and presence of exogenous metabolic activation.

Lowest concentration producing cell toxicity:

a. LD50 (no activation): 23.2 to 50 ug/ml.

b. With activation: no reduction in cell survival to 4000 ug/ml

	+	?	-
with metabolic activation:	[ ]	[ ]	[X]
without metabolic activation:	[ ]	[ ]	[X]

Comments: Concentrations for testing transformation activity:

a. No activation: 62.5 to 16.0 ug/ml.
b. With activation: 1.0 to 0.063 mg/ml

Solvent was ethanol; MMNG and DMN were positive controls.

Reference: l) Shell Development Company

2. (Cytogenetic Assay)

Test substance: 1-Octene (Netherlands)
Type of cell used: Chinese Hamster Ovary Cells
Test method (e.g., OECD, others): Chromosome aberration induction potential in CHO cells incubated in vitro, in absence and presence of activation by a rat liver microsome fraction (S-9)

GLP: YES [ ] ?
NO [ ]

Test results: 1-Octene did not induce structural chromosomal aberrations in cultured CHO cells (either in the presence or absence of S-9 mix) under the conditions of the assay.

Lowest concentration producing cell toxicity: 40 ug/ml strongly cytotoxic

	+	?	-
with metabolic activation:	[ ]	[ ]	[x]
without metabolic activation:	[ ]	[ ]	[x]

Comments: Concentrations for testing: 1.33 ug/ml to 40 ug/ml for treatment time of 3 hours. Cells were exposed to Ham's media, ethanol as solvent control, mitomycin C as positive control without activation or Cyclophosphamide as positive control with activation, or to dilutions of test article in ethanol. Harvest times were 12 and 21 hours.

Reference: p) DSM, Geleen, the Netherlands, Report No. 86.168/251124

3. (Cytogenetic assay)

Test substance: NEODENE 8 Alpha Olefin
Type of cell used: Chinese Hamster Ovary Cells
Test method (e.g., OECD, others): Chromosome aberration induction potential in CHO cells incubated in vitro, in absence and presence of activation by a rat liver microsome fraction (S-9)
GLP: YES [X]
NO [ ]

Test results:

a. No activation: Aberration rate in mean aberrations per cell and percent abnormal CHO cells from exposure to NEODENE 8 alpha olefin (collected 3, 8, and 12 hours post exposure) not significantly higher than cells exposed to solvent (95% ethanol).

b. Activation present: Treated cell aberration rate in aberrations per cell exceeded 2-fold that of solvent control at the 5 highest concentrations tested and the presence of abnormal cells exceeded 2-fold that of solvent control at 3 non-consecutive concentrations. The increases were only slightly over 2-fold the background and did not exhibit a dose response relationship.

Lowest concentration producing cell toxicity: 0.072 mg/ml
(Greater than 80% decrease in mean cell number of cells per flask as compared to solvent control, with and without activation).

	+	?	-
with metabolic activation:	[ ]	[X]	[ ]
without metabolic activation:	[ ]	[ ]	[X]

Comments:Concentrations for testing: 1.0 x 10-2 mg/ml to 1 x 10- mg/ml

Solvent was 95% ethanol; TEM and CP positive controls

Reference: m) Shell Development Company

5.6 Genetic Toxicity in vivo: No data available

5.7 Carcinogenicity: No data available

5.8 Toxicity to Reproduction: No data available

5.9 Developmental toxicity/Teratogenicity: No data available

5.10 Other:

A. Specific toxicities (Neurotoxicity, immunotoxicity, etc.)

C. Toxicodynamics, toxico-kinetics

Comments: Expected metabolism of C_8, C_{10} and C_{12} n-1-olefins: Metabolism occurs in hepatic endoplasmic reticulum via initial formation of a transient epoxide. It is further metabolized to the corresponding glycol or conjugated with glutathione. The latter two metabolites are finally excreted in urine.

Reference: Maynert et al. (1970); Oesch (1973); Shell (1990); Watabe and Maynert (1968); Watabe and Yamada (1974)

5.11 Experience with Human Exposure (give full description of study design, effects of Accidental or Occupational Exposure, epidemiology)

6. References:

a) Handbook of Chemistry and Physics, 60th ed., Weast, R.C. Ed.: CRC: Boca Raton, FL, 1979; Sec. C, p. 407.

b) Lappin, G.R. and Sauer, J.D. Alpha Olefin Applications Handbook. New York: Marcel Dekker, 1989, p. 425.

c) The Merck Index, 9th ed., Merck & Co.: Rahway, NJ, 1976, p. 224.

d) Ethyl Corporation - Internal information

e) Ethyl Corporation sponsor, "Report on the Acute Toxicity of Alpha Olefin C8," Tulane University School of Medicine, June, 1973, Unpublished.

f) Shell Development Company, sponsor, Westhollow Research Center, "Acute Oral Toxicity of NEODENE-8 Alpha Olefin in the Rabbit", January, 1983.

g) Shell Development Company, sponsor, Westhollow Research Center, "Acute Dermal Toxicity of NEODENE-8 Alpha Olefin in the Rabbit", January, 1983.

h) Shell Development Company, sponsor, Westhollow Research Center, "Primary Skin Irritation of NEODENE-8 Alpha Olefin in the Rabbit", January, 1983.

i) Shell Development Company, sponsor, Westhollow Research Center, "Eye irritation of NEODENE-8 Alpha Olefin in the Rabbit", January, 1983.

j) Shell Development Company, sponsor, Westhollow Research Center, "Guinea pig Skin Sensitization of NEODENE-8 Alpha Olefin in the Rabbit", January, 1983.

k) Shell Development Company, sponsor, Westhollow Research Center, "Assay of NEODENE-8 Alpha Olefin for Gene Mutation in Salmonella typhimurium", January, 1983.

l) Shell Development Company, sponsor, Westhollow Research Center, "Cell Transformation Assay of NEODENE-8 Alpha Olefin in the Absence and Presence of Microsomal Activation", Performed at Litton Bionetics, Inc., January, 1983.

m) Shell Development Company, sponsor, Westhollow Research Center, "In vitro Chromosome Aberration Assay in Chinese Hamster Ovary Cells of NEODENE 8 Alpha Olefin," February, 1983.

n) DSM, Beek, the Netherlands Sponsor, Civo Institutes TNO, Report No. V 86.408/251091, "Sub-chronic (90-day) Oral Toxicity Study with Octene-1 in Rats", H.P. Til et al authors, Sept. 1986, Project No. B 85- 1091.

o) DSM, Geleen, the Netherlands Sponsor, "Examination of 1-Octene for Mutagenic Activity in the Ames Test", Report No. V 85.528/250064, Author J.W.G.M. Wilmer, Project No. B85-0064/41 and 42, December, 1985.

p) DSM, Geleen, the Netherlands Sponsor, Civo Institutes TNO, Report No. V 86.168/251124, J.W.G.M. Wilmer author, "Chromosome Analysis of Chinese Hamster Ovary Cells Treated in Vitro with 1-Octene", April, 1986, Project No. B 85-1124.

q) USEPA/OPPT/EETD/EAB; EQC model output for 1-octene. David Lynch, (11/17/2000)

1-DECENE (CAS N°:872-05-9)

FULL SIDS SUMMARY:

CAS NO.: 872-05-9		**SPECIES**	**PROTOCOL**	**RESULTS**
PHYSICAL-CHEMICAL				
2.1	Melting Point	N/A	ISO 3013	-66°C
2.2	Boiling Point	N/A	N/A	172°C
2.3	Density	N/A	ISO 3675	740 kg/m^3
2.4	Vapour Pressure	N/A	N/A	0.227 kPa at 20°C (1.7 mmHg) 0.35 kPa at 25°C
2.5	Partition Coefficient (Log K_{ow})	N/A	Measured** Calculated**	>8 5.4 - 7
2.6A	Water Solubility	N/A	measured	0.115 mg/L @ 25
2.6B	pH and pK_a	-----	-----	N/A
2.7	Flashpoint	-----	ISO 2719	46°C
2.12	Oxidation: Reduction Potential	-----	-----	N/D
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		Estimated EPIWIN	$T_{1/2}$ (-OH) = 3.6 hrs $T_{1/2}$ (O_3) = 23 hrs
3.1.2	Volatilization from water	-----	Estimated EPIWIN	$T_{1/2}$ (river) = 1.2 hrs $T_{1/2}$ (lake) = 113 hrs
3.1.3	Soil Adsorption		Estimated (C_{10})	K_{oc} = 1724
3.2	Monitoring Data	-----	-----	In air = 2.3 ug/m^3 (Leningrad 1983)
3.3	Transport and Distribution		Calculated Fugacity Level Type III Level I	In Air 5 % In Water 19 % In Soil <1 % In Sediment 76 % In Air 99.2% In Water <1% In Soil <1% In Sediment <1%
3.5	Biodegradation	N/D	Closed Bottle* Modified Sturm* <u>Psuedomonas fluorescens</u> inhibition* Estimated EPIWIN Unknown	60 – 67% 28 days but over 89% consumed at day 15. 32-46% Th CO evolved in 28-d Max inhibition of 19% for conc up to 1000 mg/L Days to weeks; fast 80.9% after 28 day
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Rainbow Trout (Salmo gairdneri) Fresh water Fish Salt water Fish	Static** Predicted Using ECOSAR Predicted Using ECOSAR	96-hr LC_{50} >1,000 mg/L 96-hr LC_{50} =0.035 mg/L 96-hr LC_{50} =0.047 mg/L
4.2	Acute Toxicity to Aquatic	Daphnid	Static**	24-hr EC_{50} = 720 mg/L

CAS NO.: 872-05-9		**SPECIES**	**PROTOCOL**	**RESULTS**
	Invertebrates	(*Daphnia magna*)		48-hr EC_{50} = 480 mg/L
			Predicted Using ECOSAR	48-hr EC_{50} = 0.048 mg/L
			Other	48-hr EC_{50} = .74 mg/l
4.3	Toxicity to Aquatic Plants	Algae (*Selenastrum capricornutum*)	4-Day Growth Test**	96-hr EC_{50} = 22 mg/l
		Green Algae	Predicted Using ECOSAR	96-hr EC_{50} = 0.037 mg/l 96-hr MATC 0.031 mg/L
4.5.1	Chronic Toxicity To Fish	Fish	Predicted using ECOSAR	30-d = 0.008 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	Daphnid (*Daphnia magna*)	Predicted Using ECOSAR	16-d EC_{50} = 0.012 mg/L
4.6.1	Toxicity to Soil Dwelling Organisms (Bacteria)	-----	-----	N/D
4.6.2	Toxicity to Terrestrial Plants	-----	-----	N/D
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (including Birds)	-----	-----	N/D
TOXICOLOGY		Composition of decene in the mixture (C_{10-13},$C_{10-14,\ and}$ C_{10-16}) are undetermined		
5.1.1	Acute Oral Toxicity	Rat	N/D	LD_{50} >10 g/kg
5.1.2	Acute Inhalation Toxicity	Rat	1 and 4 hr exposure at saturation of 9.3 and 8.7 mg/l	LC_{50} > saturation concentration
5.1.3	Acute Dermal Toxicity	Rabbit	24h exposure, 14d observation	LD_{50} >10 g/kg Some erthyrema
5.2.1	Skin Irritation	Rabbit	24h exposure Observations 24, 48 and 72h.	Non-irritating
5.2.2	Eye Irritation	Rabbit	24h exposure, observations 24, 48 and 72h.	Non-irritating
5.3	Skin Sensitization	Guinea Pig	C_{10-13} OECD 406	Cracked wax AOs were not sensitizing
5.4	Repeated Dose Toxicity			No data available, see C12-C16 analog
5.5	Genetic Toxicity *In Vitro*			
A.	Bacterial Test: Ames-Reverse Mutation Assay	*Salmonella typhimurium*	OECD 471	Negative - (with and without metabolic activation)
B.	Non-Bacterial Test:	-----	-----	N/D
5.6	Genetic Toxicity *In Vivo*	-----	-----	N/D
5.8	Toxicity to Reproduction	-----	-----	N/D
5.9	Developmental Toxicity/Teratogenicity	-----	-----	N/D
5.10	Other	Rat	Used C_{6-14} alkenes	Aspiration Hazard
5.11	Experience with Human Exposure	-----	-----	N/D

N/A = not applicable N/D = not determined AO = alpha olefin

* Shop Olefin 103 = C_{10}=19%, C_{11}=30%, C_{12}= 30%, C_{13}= 21%

** Shop Olefin 103 = C_{10-11}= 30%, C_{11-12}= 31%, C_{12}=11% and C_{13}=21%

SIDS DOSSIER
1-DECENE (CAS No: 872-05-9)

SIDS PROFILE FOR 1-DECENE

1.1	CAS NO.	872-05-9
1.2	CHEMICAL NAME	1-decene
1.3	STRUCTURAL FORMULA	CH_2=CH-$(CH_2)_7$-CH_3
2.0	OTHER CHEMICAL IDENTITY INFORMATION	Alpha Olefin, NERATEN®10
3.0	SOURCES AND LEVELS OF EXPOSURE*	
3.1	PRODUCTION RANGE	0 – 500 million pounds per year in the USA. 0- 226,796 Tonnes
3.2	CATEGORIES AND TYPES OF USE	Manufactured in closed systems. Comonomer in certain olefin products: Utilized in the production of plasticizers and other items.
4.0	ISSUES FOR DISCUSSION	

Summary of Responses to the OECD Request for Available Data on HPV Chemical

1. General Information

1.01 Substance Information

A.	CAS-Number:	872-05-9
B.	Name (IUPAC):	1-decene
C.	Common synonyms:	Alpha-Decene, N-1-Decene, Decylene, N-Decylene, NERATEN®10
D.	CAS Descriptor:	
E.	EINECS-Number:	
F.	Molecular Formula:	$C_{10}H_{20}$
G.	Structural Formula:	CH_2=CH-$(CH_2)_7$-CH_3
H.	Substance Group:	Alkene
I.	Substance Remark:	
J.	Molecular Weight:	140.26

1.0.2 OECD Information

A.	Sponsor Country:	United States and Finland
B.	Lead Organization:	United States Environmental Protection Agency
	Contact Point:	Dr. Oscar Hernandez, Director RAD US Environmental Protection Agency (USEPA) Director Risk Assessment DivisionEPA/OPPTS/RAD/7403 401 M Street, SW Washington, D.C. 20460 TELEPHONE: (202) 260_1832 TELEFAX: (202) 2601216
	Lead Organization:	Finland
	Contact Point:	Ms. Jaana Heiskanen Finnish Environment Agency Chemicals Division P.O. Box 140 00251 Helsinki

C. Name of Responder:

American Chemistry Council (Higher Olefins Panel)
1300 Wilson Blvd.
Arlington, Virginia 22209, USA

Panel Manager: Doug Anderson
Telephone: (703) 741-5616
Fax: (703) 741-6091

1.1 General Substance Information

A. Type of Substance: Organic

B. Physical State: Liquid

C. Purity of Industrial Product: Varies according to the manufacturer and production process: typically min. 93 – 96 wt%

1.2 Synonyms: Alpha-Decene, N-1-Decene, Decylene, N-Decylene,

1.3 Identity of major impurities:

n-decane (CAS # 124185)	1 wt%
2-ethyl-1-octene (CAS# 5165564)	2 wt %
2-butyl-1-hexene (CAS# 6795795)	1 wt %
Water Max.	0.01 – 0.05 wt %
Peroxide Max.	1 – 3 mg/kg
Other Hydrocarbons, mainly Max. 7 wt% (main impurity)	C_9-C_{11}

Identity of other impurities may vary depending on the production process.

1.4 Additives: Essential additives (stabilizing agents, inhibitors, other additives)

1.5 Quantity:

A. USEPA non-confidential business information aggregate figures of 100 –500 million pounds reported for the following years, 1986, 1990, 1994 and 1998.

Reference: USEPA, CUS Report, 10/27/99

B. U.S.A. Given as a range for C_8 – C_{10}, C_9 rich, 100 – 500 million pounds per year

Linear Alpha olefins, especially decene, are imported into the United States but import of these compounds is not expected to be significant.

Reference: USEPA, IR-427 Update, (1990 – 1991)

C. Production levels expressed as tones per annum information on production levels should be provided in ranges (e.g., 100-1000 tonnes, etc.) per responder or country and the date for which those ranges apply should be given.
Estimate production 1990:

USA and Europe	100,000 –200,000 tonnes
Japan	1,000-10,000 tonnes
Non-OECD countries	-
Soviet Union	10,000-20,000 tonnes

Reference: Individual country submissions

1.6 Labeling and Classification:

International Transport Classification

UN Number	1993
Class	3
Packaging group	3
Hazard identity No.	30
Proper shipping Name	Flammable liquids, N.O.S. (1-decene)
CEFIC-Tremcard No.	30G35

ADR and RID (Road, Railway)	
Class	3/31 ©
Symbol	Flammable liquid
Proper shipping name	1-decene

TA/ICAO (air)	
Class	3
Packing group	3
Symbol	Flammable liquid
Proper Shipping Name	

IMO/IMDG (SEA)	
Class	3
Page	3345
EmS-No	3-07
MFAG-No	4.2
Packing group	III
Symbol	Flammable liquid N.O.S. (1-decene)

According to EC directive 67/548/EEC: not labeled/classified in the list of Dangerous Substances – manufacturers/importers have to provissionally label/classify.

1.7 Use Pattern: Information concerning uses (including categories and types of uses expressed in percentage terms)

A. Industrial uses: As intermediate in closed systems. Co-monomer in high density polyethylene production: used captively in the production of oxo alcohols for plasticizers and detergents; used captively in the production of linear alkybenzenes for detergents. Alcohol manufacture (for PVC plasticizers), detergent and synthetic fuel oils and specialty chemicals.). Examples of use categories are dyestuffs, intermediates, solvents, adhesives, building material agents, detergents, cleaning agents, fertilizers, plastic agents, surface treatment agents, etc.

Use categories: mainly production in manufacturing of poly-alpha-olefins (used e.g. in synthetic lubricants). 1-decene can also be used in production of alcohol's (used e.g., in palsticizers, detergents) and as a co-monomer in certain olefin products.

Reference: (USEPA, IR-427 Update, (1990 – 1991) and Neste (1990)[a]

B. Public Use (Consumer Products): Anticipated to be negligible however there is some evidence indicating that possible exposure may occur from gasoline products and plastics residues.

Reference: USEPA, IR-427-Update, (1990 –1991)

C. Export: No data available

1.8 Occupational Exposure Limit Value: No data available

1.9 Sources of Exposure:

Manufacturing and Processing: Primarily inhalation or dermal contact during manufacturing, formulation, transportation and use.

Processes: No measured data available. Occupational and environmental exposure is expected to be low due to handling in closed systems. Potential occupational exposure occurs via inhalation of vapors (concentrations in the ppm-range) or splashes to skin or eyes during open handling. Examples of open handling of 1-decene are: reactor operations, maintenance, loading and unloading operations.

Reference: Neste (1990)[a], Ethyl (1990)

Consumer: Not anticipated. Please see General population exposures.

General: Has been found identified in drinking water supplies.

Reference: USEPA, IR-427-Update, (1990 –1991)

General population exposure to C_6-C_{12} alkenes is probably limited to contact with low concentration of the compounds in ambient air and finished petroleum products.

Possible exposure by inhalation due to being a combustion product of automobile exhaust, gasoline products or burning plastics

Reference: CRCS, IR-427 (1985).

Possible exposure from ingestion of contaminated seafood.

Reference: USEPA, IR-427-Update, (1990 –1991)

1.10 Additional Remarks:

2. Physical –Chemical Data

2.1 Melting or Decomposition Point:

A. Method (e.g., OECD, others): ISO 3013
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: - 66 °C

Comments: Melting points mentioned in the literature (-66 °C and –66.3 °C) are equal to the freezing point given in 2.13A.

Reference: a) Clayton and Clayton (1981), b) Sax and Lewis (1987), c) Verschueren (1983),

B. Method (e.g., OECD, others): Not known
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: -66.3 °C

Comments: Melting points mentioned in the literature (-66 °C and –66.3 °C) are equal to the freezing point given in 2.13A.

Reference: d) Sorbe (1983), e) Sumitomo (1990), f) Ethyl (1990)

C. Method (e.g., OECD, others): Not known
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: -90^{0}F (pour point)

Comments: source from Chevron, MSDS.

Reference: CRCS, Inc, IR-427, (1985)

2.2 Boiling Point: (Including temperature of decomposition, if relevant)

A. Method (e.g., OECD, other): Not mentioned
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 172 °C[a] at? kPa
Comments: Boiling point may be determined for pure 1-decene, boiling ranges for product, which contains impurities.

Reference: Sax and Lewis (1987); Sorbe (1983), Verschueren (1983)

B. Method: ISO 4626 (OECD Guideline 103)
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 5% 158 °C
95% 168 °C

Reference: Shell (1990)

C. Method:ASTM D 86
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 5% 162 °C
95% 165.5°C
Reference: Chevron

D. Method:Not Mentioned
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 5% 170 °C
95% 172 °C

Reference: Lappin and Sauer

E. Method:Not mentioned
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 5% 170 °C
95% 171 °C

Reference: Sumitomo (1990)

2.3 Density:

A. Method (e.g., OECD, others): ISO 3675
GLP: Yes [ ] Not Known [ ]
No [ ]

Test Results: 740 kg/m^3 at 20 °C

Reference: Shell (1990)

B. Method (e.g., OECD, others): ASTM D 287
GLP: Yes [ ] Not Known [ ]
No [ ]

Test Results: 745 kg/m3at 15.6 °C (specific gravity)

Reference: Chevron

C. Method (e.g., OECD, others): Not known
GLP: Yes [ ] Not Known [ ]
No [ ]

Test Results: 741 kg/m3at 20 °C

Reference: Ethyl (1990)

2.3.1 Vapor Pressure

A. Method: Not mentioned
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 0.133 KPa at 14.7 °C, 0.227 Kpa at 20° C, 1.33 Kpa at 53.7 °C,

Reference: Verschueren (1983)

B. Method: Not mentioned
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 5.32 KPa at 83.3° C

Reference: Ethyl (1990)

C. Method: (graphically evaluated)
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 0.35 KPa at 25 °C

Reference: Chevron (1990)

D. Method: (calculated)
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 0.21 KPa at 25 °C

Reference: Organic Solvents, ED.4 (1986); Riddick et al.

2.5 Partition Coefficient n-Octanol/Water

A. Method : Calculated via KOWwin, W. Meyland and P. Howard ;
Input values : ws = 0.115 mg/l ; VP= 1.67 mmHg ; BP = 170.5^{o}C ;
MP = -66.3^{o}C

Test Results : log K_{ow} = 5.12

Reference: HEDSET, 01/19/95; USEPA EPIWIN/ECOSAR Program (8/99), OPPT/RAD/ECAB

B. Method: Calculated
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: Log K_{ow} = 5.0

Comments (e.g., is the compound surface active or dissociative?): Analytical Method: Calculation method for one value is published by Chiou et al. In Environmental Science and Technology 16 (1): 4-10 (1982). The source of the value is unknown. Calculation method is based on water-solubility of 1-decene, which have not been mentioned anywhere.

Reference: Ethyl (1990)

C. Method: Measured
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: Log K_{ow} = 5.7 at 25 °C

Reference: American Petroleum Institute (1994)

F. Test Substance: Shop Olefin 103; C_{10-11} – 30%, C_{11-12}= 31%, C_{12} = 11% and C_{13} = 21%

Method: Measured; reverse phase HPLC
GLP: Yes [x]
No [ ]

Test Results: Log n-octanol/water partition coefficient = >8

Comments: Indicate a high potential for Shop Olefins 103 to accumulate from water into organisms.

Reference: Shell Research Group. SBGR. 85.182.

G. Test Substance: Shop Olefin 103 C_{10-11} – 30%, C_{11-12}= 31%, C_{12} = 11% and C_{13} = 21%

Method: Calculated from chemical structure

Test Results: 5.4 – 7.0

Reference: Shell Research Group. SBGR. 85.182.

2.6 Water Solubility:

A. Method (e.g., OECD, other):
GLP: Yes [x] Not Known [ ]
No [ ]

Test Results: 0.115 mg/L at 25 °C

Reference: Shaw, D.G. (1989)

B. Method: Calculated; EPIWIN, WSKOW v 1.33
Test Results: .3066 mg/L at 25°C

Reference: USEPA, EPIWIN (8/99), OPPT/RAD/ECAB

2.7 Flash Point (Liquids)

A. Method: ISO 2719 (Pensky-Martens closed cup method, EC method)
closed cup [x] open cup [ ]
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 46 °C

Reference: Shell (1990)

B. Method: ASTM D 56 (Tag Closed Tester, EC method)
Closed cup [X] open cup [ ]
GLP: Yes [ ] Not Known [x]
No [ ]

Test Results: 48.9 °C (120 °F)

Reference: Chevron

2.8 Auto Flammability: No data available

2.9 Flammability (Solid/Gases): No data available

2.10 Explosive Properties:

Method: unknown
Test Results: Lower Explosive Limit (LEL) = 0.5%
Upper Explosive Limit (UEL) = 5.4%

Reference: Ethyl (1990)

2.11 Oxidizing Properties: No data available

2.12 Oxidation: Reduction Potential: No data available

2.13 Additional Remarks:

A. Freezing point:

Method: ISO 3013
Test Result: -66 °C
Reference: Shell 1990

B. Autoignition Temperature

a) Method: ASTM E659 (EC method)
Test Result: 210 C (410 °F)[a]

Reference: Chevron

b) Method: -----
Test Result: 235 °C

Reference: Sorbe (1983)

c) Method: Not mentioned
Test Result: 244 °C

Reference: Shell (1990)

C. Viscosity

a) Method: ISO 3104 (OECD Method 114)
Test Results: 1.1 cSt at 20 °C[a]

Reference: Shell (1990)

b) Method: Not mentioned
Test Results: 0.75 cP at 20 °C[a]

Reference: Sumitomo (1990)

c) Method: Not mentioned
Test Results: 0.728 cP at 20 °C[c]
0.491cP at 50 °C[c]

Reference: Lappin and Sauer (1989)

D. Refractive Index
Method: SMS 473
Test Results: 1.42

Reference: Shell (1990)

E. Threshold Odor Concentration in Air
Method: Not mentioned
Test Results: 1) 0.066 mg/m3 (0.011 ppm)[a]; 0.12 ppm
2) About 7 ppm[b]

Reference: a) Verschueren (1983)
b)Clayton and Clayton (1981)

F. Reactivity and corrosive properties
Reacts when exposed to catalysts producing internal olefins and/or dimers, trimers, tetramers or higher oligomers.

Contact with oxygen results to slow formation of hydroperoxides, which can decompose to carbonyl-containing impurities. UV-light increases the hydroperoxide formation. Hydroperoxides can interfere reactions of 1-decene and cause danger of explosion.

Alpha olefins will damage many rubbers, paints, and lining materials.

Comments: -
Reference: Lappin and Sauer (1989)

3. Environmental Fate and Pathways:

3.1 Stability:

3.1.1. Stability in Air: Photodegradation:
Test substance: 1-decene
Test method or estimation method (e.g., OECD, others): calculated using USEPA EPIWIN/ECOSAR, 8/99; input values mw= 140.27; ws= 0.115 ppm, vp = 1.67 mmHg, Henry's law = 2.68 atm/m^3/mol
GLP Yes [ ]
No [X]

Test results: $T_{1/2}$ (hyroxy radical) = 3.582 hrs
$T_{1/2}$ (Ozone) = 22.92 hrs

Reference: USEPA, EPIWIN/ECOSAR (8/99), OPPT/RAD/ECAB

3.1.2. Stability in Water: No data

3.1.3. Stability in Soil: Soil Adsorption
Test Substance: 1-decene
Test method or estimation method: calculated using USEPA EPIWIN/ECOSAR, 99

Test Results: Strong; Koc = 1724

Comments: May be mitigated by rapid volatilization.

Reference: USEPA, EPIWIN/ECOSAR, [10/99], OPPT/RAD/ECAB

3.2 Monitoring Data (Environment)
Test substance: 1-decene
Indicate whether the data are measurements of background concentrations or measurement at contaminated sites:

-air 0 – 8300 (ug/m3) in air above shale oil retort wastewater as of 1990 or earlier[a].

-air 2.3 (ug/m3)ambient air in Leningrad air as of 1983[a]

-air 1-decene has been detected in the exhaust gas of diesel engines.[a]

-air Detected in air samples taken from a landfill in the UK, including municipal, industrial and liquid co-disposal sites.[b]

-Indoor Air 1-decene has been found in indoor air samples from Northern Italy.[b]

-Waste water 137 ppb effluent of a specialty chemicals manufacturing[a]

- Food detected in walleye or trout taken from the Great Lakes in the USA (quantitative data not available)[a]

-Drinking Water 1-decene has been qualitatively determined to be found in drinking water and also has been identified in drinking water samples taken from the United Kingdom.[b]

-Natural Sources 1-decene has been isolated from the leaves and rhizome of the plant Farfugium japonicum[a].

Comments:

1-decene has been detected as the initial product in the microbial degradation of n-decane. 1-decene has been identified in the emissions of high altitude jet aircraft engines.

1-decene has been detected in the environment. It appears that the releases of 1-decene are occuring from secondary sources (i.e combustion) and are not a direct result of manufacturing and processing. Consumer exposure is not expected however, the potential does exist for general population exposure. It should be noted that general population exposures were not estimated since the exposure is estimated to occur from secondary sources.

Reference:

a) CRCS (1985)
b) (CRCS, IR-427 Update (1990-1991))

3.3 Transport and Distribution between environmental compartments including estimated environmental concentrations and distribution pathways.

3.3.1 Transport: Volatilization from Water

Test substance: 1-decene

Test method or estimation method (e.g., OECD, others): calculated using USEPA EPIWIN/ECOSAR, 8/99, input values mw= 140.27; ws= 0.115 ppm, vp = 1.67 mmHg, Henry's law = 2.68 atm/m^3/mol

GLP Yes [ ]
No [X]

Test results: $T_{1/2}$ (river) = 1.209 hrs for a river 1meter deep, wind velocity 5 m/sec and current 1 m/sec.

$T_{1/2}$ (lake) = 112.5 hrs for a lake 1 meter deep, wind velocity 0.5 m/sec and current 0.05 m/sec.

Reference: USEPA, EPIWIN/ECOSAR (8/99), OPPT/RAD/ECAB

3.3.2 Theoretical Distribution (Fugacity Calculations)

A. Type of transport and distribution processes between compartments

Substance: 1-decene
Method: Calculated using EQC (Mackay level III Fugacity Model)

Test Results:

Utilizing default emission values

Air	2.44%
Water	30.4%
Soil	45.4%
Sediment	22%

Utilizing estimated emission values provided by American Chemistry Council (10 kg/hr to air, 1 kg/hr to water, 0 kg/hr to soil)

Air	5%
Water	19%
Soil	<1%
Sediment	76%

Reference: USEPA/OPPT/EETD/EAB; EQC model output for 1-decene. David Lynch, (11/17/2000)

B. Substance: 1-decene
Method: Calculated using EQC (Mackay level I Fugacity Model)

Test Results:		
	Air	99.2
	Water	<1%
	Soil	<1%
	Sediment	<1%

Reference: USEPA/OPPT/EETD/EAB; EQC model output for 1-decene. David Lynch, (11/17/2000)

3.4 Mode of Degradation in Actual Use: Probably mainly aerobic biodegradation

3.5 Biodegradation:

A.

Test Substance:	Shop Olefin 103: contains: C_{10} = 19 %, C_{11}= 30%, C_{12}= 30%, C_{13} = 21%)
Test type:	aerobic [ ], anaerobic [ ]
Test medium:	Sodium benzoate used a biodegradable substance to demonstrate the activity of microbial inoculum.
Test Method:	Closed Bottle, EC Test Guideline C.4-E
GLP:	Yes [ ] No [ ]
Test Results:	Closed bottle: 60 – 67% in 28 days; but over 89% of the possible oxygen demand was consumed in the bottles titrated at day 15. There was no inhibition of microbial activity in the closed bottle test. “Readily biodegradable”
Comments:	The test substance was not wholly soluble in water at the conc used, it was supplied by degrading organisms as an emulsion in a non-biodegradable detergent, Doban PT sulphonate.
Reference:	Shell Group Research Report SBGR: 85.106 (Shell 1985)

B.

Test Substance:	Shop Olefin 103: contains: C_{10} = 19 %, C_{11}= 30%, C_{12}= 30%, C_{13} = 21%)
Test type:	aerobic [ ], anaerobic [ ]
Test medium:	Sodium benzoate was used as a degradable substance to demonstrate the activity of microbial inoculum. Controls with mineral medium and microbial inoculum we included.
Test Method:	Modified Sturm
GLP:	Yes [ ] No [ ]

	Test Results:	32-46% of the theoretical carbon dioxide being evolved in 28 days.
	Comments:	As the test compound was not wholly soluble in water at the conc used, it was supplied to the degrading organisms as an emulsion in a non-biodegradable detergent, Doban PT sulphonate.
	Reference:	Shell Group Research Report SBGR: 85.106 (Shell 1985)
C.	Test substance:	1-decene
	Test type	aerobic [x], anaerobic [x]
	Test medium:	Water
	Test method (e.g., OECD, ISO, others):	Calculated using USEPA EPIWIN/ECOSAR
	GLP:	Yes [ ] No [X]
	Test results: aerobic:	days to weeks; fast Anaerobic:weeks to months
	Reference:	USEPA, EPIWIN/ECOSAR (8/99), OPPT/RAD/ECAB
E.	Test Substance:	1-decene
	Test type,	aerobic [x], anaerobic [ ]
	Test medium:	activated sludge, domestic
	Test method:	Not stated
	GLP:	Yes [ ] No [ ]
	Test results:	
	Concentration:	18.6 mg/l related to test substance.
	Degradation:	80.9% after 28 day Readily biodegradable
	Comments:	10 day time window = day 3 to day 13; degradation at the end of the 10 day time window = 64.9% (mean), degradation at plateu = 81% (mean)
	Reference:	Enichem Instituto G Donegani- Final Report on ready biodegradability (manometric-respirometric) of olefin C_{10}. (April, 1995)

3.6 BOD-5, COD or Ratio BOD-5/COD: No data available

3.7 Bioaccumulation:

Test substance: 1-decene
Test method (e.g., OECD, others): Not known (calculation)
Type of test: Static [ ], semi-static [ ], flow-through [ ], Other (e.g., field test) [ ]

GLP: Yes [ ]
No [ ]

Test results: may bioaccumulate (Log Kow = 3 –6

Bioaccumulation factor: Calculated results: BCF = 525 (Log Kow = 3.9)
BCF = 3982 (Log Kow = 5.0)

Method of Calculation: Calculation seem to be based on the calculated log Kow – coefficients.
(see point .24)

Reference: Ethyl (1990) Referred to CRCS (1985)

3.8 Additional Remarks:

A. Sewage Treatment

Test Substance: 1-decene
Method: Calculated using EPIWIN/ECOSAR, input values mw= 140.27; ws= 0.115 ppm, vp = 1.67 mmHg, Henry's law = 2.68 atm/m^3/mol

Test Results: 99% of 1-decene was eliminated with a rotating disk aerator.
99.98% total removal

Comments: Moderate to extensive stripping to air along with moderate absorption. Biodegradation may also be a contributing factor to removal.

Reference: CRCS (1998); USEPA EPIWIN/ECOSAR (8/99) OPPT/RAD/ECAB

B. Migration to ground water

Test Substance: 1-decene
Method: Calculated using EPIWIN/ECOSAR, (8/99); input values mw= 140.27; ws= 0.115 ppm, vp = 1.67 mmHg, Henry's law = 2.68 atm/m^3/mol

Test Results: Rate – slow

Comments: May be mitigated by rapid volatilization

Reference: USEPA EPIWIN/ECOSAR (8/99); OPPT/RAD/ECAB

C. Soil Migration

Test Substance: 1-decene
Method: Calculated using EPIWIN, (8/99); input values mw= 140.27; ws= 0.115 ppm, vp = 1.67 mmHg, Henry's law = 2.68 atm/m^3/mol

Test Results: Slow

Comments: May be mitigated by rapid volatilization

Reference: USEPA EPIWIN/ECOSAR (8/99); OPPT/RAD/ECAB

D. Soil Volatilization

Test Substance: 1-decene

Method: Calculated using EPIWIN (8/99); input values mw= 140.27; ws= 0.115 ppm, vp = 1.67 mmHg, Henry's law = 2.68 atm/m^3/mol

Test Results:

Soil mobility:	low
Dry Soil:	may exist
Moist Soil:	rapidly

Reference: Swann et al, (1983) and USEPA EPIWIN (8/99); OPPT/RAD/ECAB

4. Ecotoxicological Data

4.1 Acute/prolonged toxicity to fish

A. Test substance: Shop Olefin 103 C_{10-11} – 30%, C_{11-12}= 31%, C_{12} = 11% and C_{13} = 21%
Test species: Salmo gairdneri,
Test method (e.g., OECD, others): 4-day growth test
Type of test static [x], semi-static [], flow-through [ ]
Other (e.g., field observation) [ ]
GLP: Yes [x]
No [ ]

Test results: LC50 (96-hr) = >1,000 mg/L

Comments: A 96-hr static toxicity test was carried out with daily renewal of the test solutions. At 24 hr intervals the number of dead fish were recorded and removed, dissolved oxygen concentrations and pH were measured and the test solutions renewed. The temperature of the solutions during the test was 18.5 $\pm 1.0^0$C, pH was 7.4 – 8.4, the total water hardness was 222-262 mg/l as $CaCO_3$ and the concentration of dissolved oxygen was 9.0-10.2 mg/l.

Reference: Shell Group Research Report SBGR 85.182, Shell, (1985)

B. Test substance: 1-decene
Test species: fish
Test method (e.g., OECD, others): calculated using EPIWIN/ECOSAR; input values: MW=140.27, mp = -66.3°C, log Kow = 5.7, WS = 0.115 mg/L
GLP: Yes [ ]
No [X]

Test results: Freshwater Fish LC50 (96-hr) = 0.035 ppm Saltwater Fish LC50 (96-hr) = 0.047 ppm

Reference: USEPA, EPIWIN/ECOSAR (8/99), OPPT/RAD/ECAB

4.2 Acute Toxicity to Aquatic Invertebrates - daphnids

A. Test substance: Shop Olefin 103 C_{10-11} – 30%, C_{11-12}= 31%, C_{12} = 11% and C_{13} = 21%
Test species: Daphnia magna.
Test method (e.g., OECD, others): Static Water Test
GLP: Yes [x]
No [ ]

Test results: EC50 (24 hr) = 720 mg/L
EC50 (48-hr) = 480 mg/L

Reference: Shell Research Group. SBGR. 85.182

B. Test substance: 1-decene
Test species: Daphnia magna.
Test method (e.g., OECD, others): calculated using EPIWIN/ECOSAR; input values: MW=140.27, mp = -66.3°C, log Kow = 5.7, WS = 0.115 mg/L

GLP: Yes [ ]
No [X]

Test results: LC50 (48-hr) = 0.048 ppm

Reference: USEPA, EPIWIN (8/99), OPPT/RAD/ECAB

C. Test Substance: Olefin 103 PQ11
Test Species: Daphnia magna (Crustacea)
Test Method: Other
GLP: Yes [x]
No [ ]

Test Results: 48hr EC_{50} = .74 mg/l

Comments: Nominal concentrations used. Experimental method did not use sealed vessels and test solution was aerated. Testing with C_{10-13} AO blend under the same test conditions gave a 48 hr EC_{50} = 480 mg/l (SBGR 85.182).

Based on TDS QSAR calculation decene is expected to be very toxic to Daphnia (LC_{50}= 0.9 mg/l). In view of the high tendency to evaporate from water the substance is unlikely to pose a hazard to aquatic organisms.

Reference: Garforth, B., Olefins 103 PQ11: Acute Toxicity to Salmo gairdneri, Daphnia magna and Selenastrum capricornutum, Sittingborne report 83.359, 1983.

Pearson, N., Shop Olefins 103: Acute toxicity (Salmo gairdneri, Daphnia magna, Selenastrum capricornutum) and n-octano/water partition coefficient, Sittingborne report, SBGR 85.182, 1985.

4.3 Toxicity to Aquatic Plants, e.g. algae

A. Test substance: Shop Olefin C_{10-11} – 30%, C_{11-12}= 31%, C_{12} = 11% and C_{13} = 21%
Test species: *Selenastrum capricornutum*
Test method (e.g., OECD, others): 4 day Growth Test
GLP: Yes [x]
No [ ]

Test results: 96-hr EC50 based on cell numbers at day 4 was calculated to be 22 mg/L

Reference: Shell Research Group, SBGR. 85.182,

B. Test substance: 1-decene
Test species: algae
Test method (e.g., OECD, others): calculated using EPIWIN/ECOSAR; input values: MW=140.27, mp = -66.3°C, log Kow = 5.7, WS = 0.115 mg/L
GLP: Yes [ ]
No [X]

Test results: EC_{50} (96 hr) = 0.037 ppm
Chv (96-hr) = 0.031 ppm

Reference: USEPA, EPIWIN/ECOSAR (8/99), OPPT/RAD/ECAB

4.4 Toxicity to Bacteria:

Test Substance:	Shop Olefin 103: contains: C_{10} = 19 %, C_{11}= 30%, C_{12}= 30%, C_{13} = 21%)
Test type:	aerobic [ ], anaerobic [ ]
Test medium:	Pseudomonas fluorescens , Sodium pentachlorophenate was used as a standard inhibitory substance.
Test Method:	Inhibition of Growth
GLP:	Yes [ ] No [ ]
Test Results:	Maximum inhibition of growth of 19% for conc up to 1000 mg/L
Reference:	Shell Group Research Report SBGR: 85.106 (Shell 1985)

4.5 Chronic Toxicity to Aquatic Organisms:

4.5.1 Chronic Toxicity to Fish:

Test substance:	1-decene
Test species: fish	
Test method (e.g., OECD, others): calculated using EPIWIN/ECOSAR; input values: MW=140.27, mp = -66.3°C, log Kow = 5.7, WS = 0.115 mg/L	
GLP:	Yes [ ] No [X]
Test results:	LC_{50} (14 day) = 0.113 ppm Chv (30 day) = 0.008 ppm
Reference:	USEPA, EPIWIN (8/99), OPPT/RAD/ECAB

4.5.2 Chronic Toxicity to Aquatic Invertebrates:

Test substance:	1-decene
Test species:	daphnia
Test method (e.g., OECD, others): calculated using EPIWIN/ECOSAR; input values: MW=140.27, mp = -66.3°C, log Kow = 5.7, WS = 0.115 mg/L	
GLP:	Yes [ ] No [X]
Test results:	EC_{50} (16 day) = 0.012 ppm
Reference:	USEPA, EPIWIN/ECOSAR (8/99), OPPT/RAD/ECAB

4.6 Toxicity to Terresterial Organisms: No data available

4.6.1 Toxicity to soil dwelling organisms: No data available

4.6.2 Toxicity to terrestrial plants: No data available

4.6.3 Toxicity to other Non-Mammalian Terrestrial Species (birds):
No data available

4.7 Biological Effects Monitoring: No data available

4.8 Biotransformation and Kinetics:No data available

4.9 Additional Remarks:

5. Toxicological Data

5.1 Acute toxicity

5.1.1 Acute oral toxicity

A.
Test substance: 1-decene
Test species/strain: 10 albino male Wistar rats
GLP Yes [ ] Not Known [x]
No[ ]

Test results: LD50> 10 g/kg

Comments: 1-decene manufactureres are requested to add the missing original references, where possible.

Reference: Rinehart (1967)

B.
Test substance: 1-decene
Test species/strain: Rat/Strain not mentioned
GLP Yes [ ] Not Known [x]
No[ ]

Test Results: LD50> 10 g/kg
$C_{10} - C_{13}$ alpha olefins: LD50 (rat) 7.7 g/kg[b]

Reference: Shell (1990)

C.
Test substance: 1-decene
Test species/strain: Rat/Strain not mentioned
GLP Yes [ ] Not Known [x]
No[ ]

Test Results: LD50> 10 g/kg

Reference: Sumitomo (1990)

D.
Test substance: 1-decene
Test species/strain: Rat/Strain not mentioned
Test method (e.g., OECd, limit test, fixed dose test): one dose, 14 days observation.
GLP Yes [ ]
No [X]

Test Results: LD50> 10g/kg. No signs of toxicity.

Comments: Testing Year- 1973.

Reference: Ethyl (1990)

E.
Test Substance: $C_{10} - C_{14}$ alpha olefin (blend not specified)
Test Species: Rats and Mice
GLP Yes [ ]
No [x]

Test Results: LD50 or other measure of acute toxicity (e.g., in case of fixed-dose text
21.3 g/kg(rat); 17.3 g/kg (Mouse)

Reference: Abasov, D.

5.1.2 Acute Inhalation Toxicity

A. Test substance: 1-decene
Test Species/Strain: Rat/Strain not mentioned
Test method (e.g., OECD, limit test, fixed dose test): Not mentioned
GLP Yes [ ] Not Known [x]
No [ ]

Test Results: No mortality at 320 ppm or vapor for one hour

Comments: the references in A and B of the LC50-value of 1-decene may be based on the same original test.

Reference: Rinehart (1967)
a)Shell (1990)

B. Test substance: 1-decene
Test Species/Strain: Rat/Strain not mentioned
Test method (e.g., OECD, limit test, fixed dose test):Not mentioned.
GLP Yes [ ] Not Known [x]
No [ ]

Test Results: LC50 (1 hour) > 320 ppm (1860 mg/m^3)[a]

Other data: Shop Olefins 103 C_{10} - C_{13} alpha olefins (blend not specified): LC50 (4 hour, rat) > 2.1 mg/L[b]

Comments: the references from A and B of the LC50-value of 1-decene may be based on the same original test.

Reference: (a) Shell (1990)
(b) Shell Research Limited: Group Research Rpt TLGR.80.052; The Acute Inhalation Toxicity of Olefins 103 PQ11

C. Test substance: 1-decene
Test Species/Strain: Rat/Sprague Dawley
Test method (e.g., OECD, limit test): 1 and 4 hours exposure at saturation of 9.3 and 8.7 mg/L (g/m^3) (Calculation 2270 ppm).
GLP Yes [ ]
No [X]

Test results: LC50> Saturation concentration

Comments: No visible pathological changes seen after 14 days. No lethality. Human experience indicates that inhalation may cause CNS depression. Testing year 1973.

Reference: Ethyl (1990)

5.1.3. Acute dermal toxicity

A. Test substance: 1-decene
Test Species/Strain: Rabbit/Strain Not mentioned
Test method (e.g., OECD, limit test): Not mentioned
GLP Yes [ ] Not Known [x]
No [ ]

Test results: LD50 > 10 g/Kg, Deleted local hairloss and skin damage.

Reference: Rinehart (1967)

B. Test substance: 1-decene
Test Species/Strain: Rabbit/Strain Not mentioned
Test method (e.g., OECD, limit test): Not mentioned
GLP Yes [ ] Not Known [x]
No [ ]

Test results:
$C_{10} - C_{13}$ alpha olefins: LD50 (rat) = 3.0 g/kg

Reference: Shell (1990)

C. Test substance: 1-decene
Test Species/Strain: Rabbit/Strain Not mentioned
Test method (e.g., OECD, limit test):Not mentioned
GLP Yes [ ] Not Known [x]
No [ ]
Test results:
LD50 > 10 g/Kg,

Reference: Sumitomo (1990)

D. Test substance: 1-decene
Test Species/Strain: Rabbit/New Zealand White
Test method (e.g., OECD, limit test): 24 hour exposure, 14 days observations
GLP Yes [ ] Not Known [x]
No [ ]
Test results: LD50 > 10 g/kg, some erythema

Comments: Testing year 1973[d]
Reference: Ethyl (1990)

5.2 Corrosiveness/Irritation

5.2.1 Skin Irritation

A. Test substance: 1-decene
Test Species/Strain: Rabbit/Strain Not mentioned
Test method (e.g., OECD, others): Draize test (OECD 404)
GLP: Yes [ ] Not Known [x]
No [ ]

Test results: Give maximum scores after….hrs. Maximum individual score = 4.0/8.0 at 72 hours.
24 hours Draize: Primary skin irritation index 0.9 (non-irritating)

Comments: 1-decene manufacturers are requested to add the missing testing data, where possible.

Reference: Rinehart (1967)

B. Test substance: Alpha Olefin PQ11 103; C_{10-11} = 37%, C_{11-12}=31%, C_{12} =11%, C_{13}=21% Test Species/Strain: Rabbit/Strain Not mentioned
Test method (e.g., OECD, others): Draize test (OECD 404)
GLP: Yes [ ] Not Known [x]

No [ ]

Test results: $C_{10} - C_{13}$ cracked wax alpha olefins: Severely irritating (24 hour Draize test, rabbit)

Comments: Although $C_{10} - C_{13}$ cracked wax alpha olefins have been severely irritating in Draize Test, the specific data of 1-decene is regarded as more valid.

1-decene manufacturers are requested to add the missing testing data, where possible.

Reference: (7) Shell (1990), Toxicology of AO: Acute Toxicity, Skin and Eye Irritatancy and Skin Sensitizing Potential of AO 103 PQ11.

C. Test substance: Gulftene 10
Test Species/Strain: New Zealand White Rabbit
Test method (e.g., OECD, others): Draize test (OECD 404)
GLP: Yes [X]
No [ ]

Test results: Primary Irritation index of 3.67
Mean scores of 2.0 erythema/eschar formation and 1.7 for oedema

Comments: No corrosive effects were noted

Reference: Chevron, Gulftene 10, Acute Dermal Irritation Test in the Rabbit, SPL Project Number: 703/077 (1996)

D. Test substance: Alpha Olefin PQ11 103; C_{10-11} = 37%, C_{11-12}=31%, C_{12} =11%, C_{13}=21% Test Species/Strain: Rabbit/Strain Not mentioned
Test method (e.g., OECD, others): Semi-occluded patch test (ST-SOP 229)
GLP: Yes [X]
No [ ]

Test results: Group mean 24, 48 and 72 hour
Erythema: 1-7
Oedema: 0.5
Moderately Irritating

Reference: Shell (1985), Toxicology of Shop Alpha Olefins: The Skin Irritancy of Shop Alpha Olefin, C_6, Shop Alpha Olefin C_{18} and Shop Olefins 103. SBGR.85.166

5.2.2. Eye Irritation

A. Test substance: 1-decene
Test species/strain: Rabbit/Not mentioned
Test method: Draize test (OECD 405).
GLP Yes [ ] Not Known [X]
No [ ]

Test results: Max individual score = 2/110 at 24 hours.; 0.7 (Max eye irritation score) (non-irritating)

Comments: 1-decene manufacturers are requested to add the missing testing data, where possible.

Reference: Rinehart (1967)

B. Test Substance: $C_{10} – C_{13}$ cracked wax alpha olefins
Test species/strain: Rabbit/strain not mentioned
Test Method: Draize test (OECD 405)
GLP Yes [ ] Not Known [X]
No [ ]

Test results: $C_{10} – C_{13}$ cracked wax alpha olefins; practically non-irritating (Draize test, rabbit)

Reference: Shell (1990)

C. Test Substance: 1-decene
Test species/strain: Rabbit/New Zealand white
Test Method: 24 hr exposure; 24 hr and 72 hr observations
GLP Yes [ ] Not Known [X]
No [ ]

Test Results: All scores 0.0 (non-irritating)

Comments: Testing year 1973.

Reference: Ethyl (1990)

5.3 Skin Sensitization

A. Test substance: C10 – C13 cracked wax alpha olefins, AO 103 PQ 11
Test Species/strain: guinea pig
Test Method: Magnusson and Kligman maximization technique, (OECD Guideline 406).
GLP: Yes [ ]
No [X]

Test Results: C10 – C13 cracked wax alpha olefins were non-sensitizing to guinea pigs

Reference: Shell (12/77), Group Research Report TLGR.0171.77, Toxicology of AP: Acute Toxicity, Skin and Eye Irritancy and Skin Sensitizing Potential of AO 103 PQ 11.

B. Test Substance: AO 103 PQ 11
Test Species/strain:

5.4 Repeated dose toxicity: No data available.

5.5 Genetic toxicity

A. Bacterial test

1. Test substance: 1-decene (manufactured by Schuchard)
Test species/strain: *Salmonella typhimurium*/TA 100, TA 98, TA 1535, TA 1538 without Enzymatic activation; TA 100 and TA 98 with S9 mix.
Test method (e.g., OECD, others): Ames method (OECD Guideline 471)
GLP Yes [x] Not Known [ ]
No [ ]

Test results: No mutagenic properties were found. 1-decene had toxic properties on TA 100 and TA 1538 without enzymatic activation

	+	?	-
With metabolic activation:	[ ]	[ ]	[x]
Without metabolic activation:	[ ]	[ ]	[x]

Reference: Burghardtova et al. (1984)

2. Test substance: 1-dodecene and C_{11}- C_{12} internal olefins
Test species/strain*: Salmonella typhimurium, Escherichia coli* and *Saccharomyces cerevisiae*
Test method (e.g., OECD, others): Unknown
GLP Yes [x] Not Known [ ]
No [ ]

Test results: 1-dodecene and C_{11}- C_{12} internal olefins did not increase reverse gene mutation frequency in in vitro test in Salmonella typhimurium and Escherichia coli. No effect on gene conversation in *Saccharomyces cerevisiae*.

Reference: Shell (1990)

3. Test substance: 1-decene
Test species/strain Salmonella typhimurium/TA 100, TA 98, TA 1535, TA 1538
Test method (e.g., OECD, others): Ames method (OECD Guideline 471)
GLP: Yes [ ] Not Known [x]
No [ ]

Test results: Toxic effects in strains TA 100 and TA 1538 (250 ug/plate) without metabolic activation.
Minimum concentration of test substance at which toxicity to bacteria was observed:

With metabolic activation: 1 – 500 ug/plate
Without metabolic activation:

Concentration of the test compound resulting in precipitation:

Genotoxic effects:

	+	?	-
With metabolic activation:	[ ]	[ ]	[x]
Without metabolic activation:	[ ]	[ ]	[x]

Comments: Results resemble reference Burghardtova et al. (1984) (see previous point 6.5.1) and may therefore be based on the same study.

Reference: CRCS (1985)

B. Non-bacterial *in vitro* test: No data available

5.6. Non-bacterial *in vivo* test: No data available

5.7 Carcinogenicity: No data available

5.8 Toxicity to Reproduction: No data available

5.9 Developmental Toxicity/Teratogenicity : No data available

5.10 Other:

A. Specific toxicity (Neurotoxicity, immunotxicity etc.):

Comments: When ingested, 1-decene is readily aspirated into the lungs if vomiting occurs. Risk of chemical pneumonitis.

Reference: Gerarde and Linden (1963)

B. Toxicodynamics, toxico-kinetics

Comments: Expected metabolism of C_8, C_{10} and C_{12} n-1-olefins: Metabolism occurs in hepatic endoplasmic reticulum via initial formation of a transient epoxide. It is further metabolized to the corresponding glycol or conjugated with glutathione. The latter two metabolites are finally excreted in urine.

Reference: Maynert et al. (1970); Oesch (1973); Shell (1990); Watabe and Maynert (1968); Watabe and Yamada (1974)

5.11 Experience with Human Exposure: No data available.

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USEPA/OPPT/EETD/EAB; EQC model output for 1-decene. David Lynch,(11/17/2000)

The references marked with the symbol "x" have been available to the Finnish Scientific Expert Group.

1- DODECENE (CAS N°: 112-41-4)

FULL SIDS SUMMARY:

CAS NO.: 112-41-4		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point	N/A	ISO 3013	-35.2°C
2.2	Boiling Point	N/A	N/A	213.8 at 20°C at 101.3 kPa
2.3	Density	N/A	N/A	0.795 g/cm^3 at 20°C 0.758 g/cm^3 0.755 -.765 g/cm^3
2.4	Vapor Pressure	N/A	Unknown	0.014 kPa @ 20°C 0.021 kPa @ 25°C 0.16 mm Hg @ 25°C
2.5	Partition Coefficient (Log K_{ow})	-----	C_{10-13} AO: (a) calculated (b) measured (c) calculated (C_{12})	 (a) Log K_{ow} = 5.4 - 7.0 (b) Log K_{ow} > 8 (c) Log K_{ow} = 6.1
2.6A	Water Solubility	-----	Unknown Estimated	(a) insoluble in water (b) 0.113 mg/L
2.6B	PH/pKa	-----	-----	N/D
2.12	Oxidation: Reduction Potential	-----	-----	N/D
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation	-----	Estimated AOP Program	$T_{1/2}$(air) OH^- = 3.3 hrs $T_{1/2}$ (air) O_3 = 22.92 hrs
3.1.2	Volatilization from Water	-----	Estimated Hydrowin Program	$T_{1/2}$ (river) = 3.8 hrs $T_{1/2}$ (lake) = 5.1 days $T_{1/2}$ (pond) = 17 months
3.1.3	Soil Adsorption		Estimated	Koc = 5864
3.2	Monitoring Data	-----	-----	N/D
3.3	Transport and Distribution		Calculated Fugacity Level Type III Level I	In Air 3 % In Water 12% In Soil <1% In Sediment 85 % In Air 85% Water <1% Soil 14.7% Sediment <1%
3.5	Biodegradation	N/D	Shop Olefin 103[1] Closed Bottle Test Shop Olefin 103[1] Modified Sturm Shop Olefin 103[1] Microbial Inhibition <u>Pseudomonas fluorescens</u> Estimated, EPIWIN	60 – 67% 28 days but over 89% consumed at day 15. 32-46% Th CO evolved in 28-d Max inhibition 19% for conc up to 1000 mg/L. Weeks

CAS NO.: 112-41-4		SPECIES	PROTOCOL	RESULTS
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Rainbow Trout (*Salmo gairdneri*)	Shop Olefin 103[2] Static	96-hr LC_{50} >1,000 mg/L
		Fish (fresh water)	Predicted ECOSAR	96-hr LC_{50} =0.017 mg/L
		Fish (salt water)	Predicted ECOSAR	96-hr LC_{50} =0.029 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates	Daphnid (*Daphnia magna*)	Shop Olefin 103[2] Static	24-hr EC_{50} = 720 mg/L 48-hr EC_{50} = 480 mg/L
			Predicted Using ECOSAR	48-hr EC_{50} = 0.025 mg/L 16-d EC_{50} = 0.008 mg/L
4.3	Toxicity to Aquatic Plants	Algae (*Selenastrum capricornutum*)	Shop Olefin 103[2] 4-Day Growth Test	96-hr EC_{50} = 22 mg/l
		Green Algae	Predicted Using ECOSAR	48-hr EC_{50} = 0.020 mg/L 96-hr EC_{50} = 0.021 mg/l 16-d EC_{50} = 0.008 mg/L
4.4	Toxicity to (Bacteria)	-----	-----	N/D
4.5.1	Chronic Toxicity To Fish	Fish	Predicted using ECOSAR	30-d = 0.004 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	Daphnia	Predicted using ECOSAR	96 hr = 0.014 mg/L
4.6.1	Toxicity to Soil dwelling Organisms	-----	-----	-----
4.6.2	Toxicity to Terrestrial Plants	-----	-----	N/D
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (including Birds)	-----	-----	N/D
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	(a) Rat	(a) 103 PQ11[3]	(a) LD_{50} >7.7 g/kg
		(b) Rat and Mouse	(b) C_{10-14} AO[4]	(b) LD_{50} = 21.3 g/kg (rat); LD_{50} = 17.3 g/kg (mouse)
		(b) Rat	(c) C_{12-16} AO[4]	(c)LD_{50} >10 g/kg
		(d) Rat	(d) C_{12} AO	(d) LD_{50} >10 g/kg
5.1.2	Acute Inhalation Toxicity			Saturated Concentrations:
		(a) Rat	(a) 103 PQ11[3]	(a) LC_{50} (4 hr) = >2.1 mg/l
		(b) Mouse	(b) C_{10-14} AO[4]	(b)LC_{50} = 223 mg/l
		(c) Rat	(c) C_{12-16} AO[4]	(c) 9900 mg/m^3; mist; 1-hour; no deaths
5.1.3	Acute Dermal Toxicity	(a) Rat	(a)103 PQ11[3]	(a) LD_{50} > 3.04 g/kg
		(b) Rabbit	(b) C_{10-14} AO[4]	(b) LD_{50} > 10 g/kg
		(c) N/D	(c) C_{12-16} AO[4]	(c) LD_{50} > 10 g/kg
	Skin Irritation	(a) Rabbit	(a) 103 PQ11[3]	(a) Single 24hr application: Severly irritating
		(b) Rabbit	(b) Shop Olefin 103	(b) Draize = 2.3/8 at 48 & 72 hours
		(c) Rabbit	c) C_{12-16} AO[4]	(c) Draize = total avg 0.4,

CAS NO.: 112-41-4		SPECIES	PROTOCOL	RESULTS
				slightly irritating.
		(d) Rabbit	(d) C_{12} AO	(d) Draize = Primary irritation index of 4.67; moderate to severe erythema and slight to severe oedema; reversible on day 14.
		(e) Rabbit	(e) C_{12}	(e) Draize = 0.1
	Eye Irritation	(a) Rabbit	(a) C_{10-13} AO[4]: Draize Method	(a) Mean score for conjunctival redness <0.33. Non-irritating per US OSHA and EU criteria:
		(b) Rabbit	(b) C_{10-14} AO[4]: Non-Standard	(b) Non-irritating per US OSHA and EU criteria:
		(c) Rabbit	(c) C_{12-16} AO[4]: Non-Standard	(c) Non-irritating per US OSHA and EU criteria:
		(d) Rabbit	(d) C_{12} AO: Non-Standard	(d) Non-irritating per US OSHA and EU criteria:
	Skin Sensitization	(a) Guinea Pig,	(a) C_{10-13} AO[4]: Magnussen &Kligman	(a) Not a skin sensitizer
		(b) Guinea Pig	(b) C_{12-16} AO[4]: Modified Landsteiner@	(b) Not a skin sensitizer
5.4	Repeated Dose Toxicity	Rat	2-Week dermal toxicity study using C12-C16 alpha olefin blend	NOAEL (systemic) = 1 g/kg/d. Repeated dermal application at 2 g/kg caused severe skin reactions and depressed body weight gains.
5.5	Genetic Toxicity *In Vitro*			
A.	Bacterial Test:			
	Ames-Reverse Mutation Assay	*S. typhimurium* and *E. coli*	C_{11-12} AO[4]	Negative with and w/out activation
	Ames-Reverse Mutation	*S. typhimurium* and *E. coli*	C_{12} AO	Negative with and w/out activation
B.	Non-Bacterial Test:			
	Mitotic Gene Conversion Assay	*S. cerevisiae*	C_{11-12} AO	Negative with and w/out activation
	Mitotic Gene Conversion Assay	*S. cerevisiae*	C_{12} AO	Negative with and w/out activation
	Chromosomal Aberration Assay	Rat Liver RL1 Cells	C_{12} AO	Negative
	Chromosomal Aberration Assay	Rat Liver RL4 Cells	C_{11-12} AO[4]	Negative
	CHO/HGPRT	Chinese Hamster Ovary	Gulftene 12-16[4]	Negative with and w/out activation
	Cell Transformation	BALB/3T3 Mouse embryo	Gulftene 12-16[4]	Negative
	Unscheduled DNA Synthesis		Gulftene 12-16[4]	Negative
5.6	Genetic Toxicity *In Vivo*	Mouse Micronucleus	Gulftene 12-16[4]	There were no remarkable

CAS NO.: 112-41-4		**SPECIES**	**PROTOCOL**	**RESULTS**
		Bone Marrow Test (dermal)		clinical findings. No significant increase in weight gain. No significant increase in micronucleated bone marrow erythrocytes or dose-related response.
5.8	Toxicity to Reproduction	-----	-----	N/D
5.9	Developmental Toxicity/Teratogenicity	-----	-----	N/D
5.10	Specific Toxicity	-----	-----	N/D
5.11	Experience with Human Exposure	-----	-----	N/D
5.12	Other Studies:	Rat	C_{12} AO and other alkenes	Aspiration Hazard

N/A = not applicable N/D = not determined AO = alpha olefin

Notes
1. Shop Olefin 103 = C_{10} = 19%; C_{11}= 30%; C_{12}= 30%; C_{13}= 21%
2. Shop Olefin 103 = C_{10-11}= 37%; C_{11-12}= 31%; C_{12} = 11%, C_{13} = 21%
3. C_{10-13} AO Blend, % Composition Unkown
4. % Composition Unknown

SIDS DOSSIER
1-DODECENE (CAS No:112-41-4)

SIDS PROFILE

1.1	CAS NO.	112-41-4
1.2	CHEMICAL NAME	1-DODECENE
1.5	STRUCTUAL FORMULA	CH_2=CH-$(CH2)_7$-CH_3
	OTHER CHEMICAL IDENTITY INFORMATION	COMMON SYNOYMS: DECYLENE C_{12} ALPHA OLEFIN NERATENE®12
3.0	SOURCES AND LEVELS OF EXPOSURE	SOURCES: CLOSED INDUSTRIAL SYSTEMS NO MEASURED DATA ON EXPOSURE
3.1	PRODUCTION RANGE	100 – 500 MILLION POUNDS
3.3	CATEGORIES AND TYPES OF USE	INDUSTRIAL USE IN CLOSED SYSTEMS MAINLY IN PRODUCTION OF POLY-ALPHA OLEFINS, OTHER USES IN PRODUCTION OF ALCOHOLS AND AS A CO-MONOMER IN CERTAIN OLEFIN PRODUCTS
ISSUES FOR DISCUSSION (IDENTIFY, IF ANY	SEE PROPOSED TESTING FOR 1-HEXENE, 1-OCTENE, 1-DECENE AND 1-TETRADECENE.	

SIDS SUMMARY

CAS NO: 121-41-4 1-dodecene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
PHYSICAL-CHEMICAL								
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	?	?	Y	N
2.3	Vapour Pressure	Y	N	N	?	?	Y	N
2.4	Partition Coefficient	Y	N	N	Y	Y	Y	N
2.5	Water Solubility	Y	N	N	N	Y	Y	N
OTHER STUDIES RECEVED								
2.6	Flash Point	Y	N	N	Y	N	Y	N
2.7	Flammability	Y	N	N	?	?	Y	N
2.9	Density	Y	N	N	Y	Y	Y	N
ENVIRONMENTAL FATE/ BIODEGRADATION								
3.5	Aerobic Biodegradability	Y	Y	N	Y	Y	Y	N
3.5	Abiotic Degradability	N						
3.1.2	Hydrolysis	Y	N	N	N	Y	Y	N
3.1.1	Photodegradability	Y	N	N	N	Y	Y	N
3.3	Env. Fate/Distribution	Y	N	N	N	Y	Y	N
	Env. Concentration	N						
OTHER STUDIES RECEIVED ECOTOXICOLOGY								
4.1	Acute Toxicity Fish	Y	Y	N	Y	Y	Y	N
4.2	Acute Toxicity Daphnia	Y	Y	N	Y	Y	Y	N
4.3	Toxicity to Algae	Y	Y	N	Y	Y	Y	N
4.4	Toxicity to Bacteria	N	N	N	N	N	Y	N
4.5.2	Chronic Toxicity to							
	- Daphnia	Y	N	N	N	Y	Y	N
	- Algae	Y	N	N	N	Y	Y	N
	- Fish	Y	N	N	N	Y	Y	N
4.6.1	- Terrest. Organisms	N						
4.6.2	- Terrest. Plants	N						
4.6.3	- Avians	N						
4.6.4	Avian Reproduction	N						
OTHER STUDIES RECEIVED TOXICOLOGY								
5.1.1	Acute Oral	Y	N	N	Y	N	Y	N
5.1.2	Acute Inhalation	Y	N	N	Y	N	Y	N
5.1.3	Acute Dermal	Y	N	N	Y	N	Y	N
5.2.1	Corrosivity, Irritation	Y	Y	N	Y	N	Y	N
5.2.2	Eye Irritation	Y	N	N	Y	N	Y	N
5.3	Skin Sensitization	Y	N	N	Y	N	Y	N
5.4	Repeated Dose	Y	Y	N	Y	N	Y	N

CAS NO: 112-41-4 1-Dodecene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
5.5	Genetic Toxicity							
	- Gene Mutation	Y	Y	N	Y	N	Y	N
	- Chromosomal Aberrations	Y	Y	N	Y	N	Y	N
5.8	Reproductive Toxicity	N	N	N	N	N	Y	N
5.12	Metabolism	N	N	N	N	N	Y	N
OTHER STUDIES RECEIVED								

Summary of Responses to the OECD Request for Available Data on HPV Chemicals

1. GENERAL INFORMATION

1.01 Chemical Identity

A.	CAS-Number:	112-41-4
B.	Name (IUPAC):	1-Dodecene
C.	Common synonyms:	Dodecene; Adacene 12;Alpha-Dodecene;N-Dodec-1-ene; Alpha-Dodecylene
D.	CAS Descriptor:	N/A
E.	EINECS-Number:	203-968-4
F:	Molecular Formula:	C_{12} H_{24}
G.	Empirical Formula:	C_{12} H_{24}
H.	Structural Formula:	$CH_2 = CH – (CH_2)_9$-CH
I.	Substance Remark:	
J.	Purity of Industrial Product:	
K.	Molecular Weight:	168.33

1.02 OECD Information

A.	Sponsor Country:	United States
B.	Lead Organization: Contact Point:	United States Environmental Protection Agency Dr. Oscar Hernandez, Director RAD US Environmental Protection Agency (USEPA) Director Risk Assessment DivisionEPA/OPPTS/RAD/7403 1201 Constitution Ave, NW Washington, D.C. 20460 TELEPHONE: (202) 564-7649 TELEFAX: (202) 564-7450
C.	Name of Responder:	American Chemistry Council (Higher Olefins Panel) 1300 Wilson Blvd. Arlington, Virginia 22209, USA Panel Manager: Doug Anderson Telephone: (703) 741-5616 Fax: (703) 741-6091

1.1 General Substance Information

A. Type of Substance: Organic

B. Physical State: (at 20EC and 1.013 hPa)
Gaseous[ ]; liquid [x]; solid [ ]

C. Purity of industrial product: Typically 95 to 97 wt % pure; purity varies according to manufacturer and production process

1.2 Synonyms: Dodecene; Adacene 12;Alpha-Dodecene;N-Dodec-1-ene; Alpha-Dodecylene

1.3 Impurities: Identity of major impurities: Impurities at >1 wt.% can include other olefins, mainly C_{10} and C_{14}; C_{12} branched isomers (mostly vinylidene) and C_{12} linear internals, random distribution.

1.4 Additives: Essential additives (stabilizing agents, inhibitors, other additives), if applicable: Storage under nitrogen atmosphere is commonly used in order to prevent contamination with air.

Reference: Lappin, G. [Reference 1]

1.5 Quantity: USEPA production volume ranges are 100 – 500 million pounds for 1986, 1990, 1994 and 1998

Reference: USEPA, CUS Report for Alpha Olefins, 10/99.

Estimated production 1992:

USA	100,000 - 150,000 Tonnes
Europe	20,000 - 30,000 Tonnes
Japan	1,000 - 5,000 Tonnes
Non-OECD Countries:	
Soviet Union	1,000 - 5,000 Tonnes

Estimated Production 1977:

USA: 60 – 150 million pounds (1977 TSCA Inventory)

1.6 Labeling and Classification:
International Transport Classification

Class	3
Packaging group	
Hazard identity No.	
Proper shipping Name	1-dodecene

CEFIC-Tremcard No.

ADR and RID (Road, Railway) 1993

Class	3,32 C
Symbol	
Proper shipping name	Alpha Olefin C_{12}
Combustible liquid	N.O.S. (1-dodecene) 3, 32 C ADR

IATA/ICAO (air)

Class	Unregulated
Packing group	
Symbol	
Proper Shipping Name	

IMO/IMDG (SEA)

Class	Unregulated
Page	
EmS-No	
MFAG-No	

Packing group
Symbol

EEC/ Labelling	Recommendation
R-phrases	None
S-phrases	None

1.7 Use Pattern:

Main Industrial Use: as intermediates in closed systems. Mainly used for production of detergent alcohols. Also used for amine production (as surfactants, other types of additives for industrial uses), ASA co-monomer, and chlorinate olefins.

1.8 Occupational Exposure Limit Value:

1.9 Sources of Exposure: No measured data available. Occupational and environmental exposure expected to be low due handling in closed systems.

Reference:

1.10 Additional Remarks: Options for disposal: Incineration, diversion to other hydrocarbons uses

2. PHYSICAL-CHEMICAL DATA

2.1 Melting Point or Decomposition Point:

Method (e.g., OECD, others) ISO 3013
GLP Yes[ ]
No [x]

Test Result: -35.2 deg C
Decomposition
Sublimation

Comments: Figure quoted is freezing point

References:
(a) U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II Washington, D.C.: U.S. Government Printing Office, 1984-5. [Reference 5]
(b) Lide, D. [Reference 2]

2.2 Boiling Point (Including temperature of decomposition, if relevant);

A. Method other: Unknown
GLP Yes[ ]
No[x]

Test Result: 213.8 deg C at 101.3 kPa

Reference: (a)Lide, D. [Reference 2]

B. Method other: Unknown
GLP Yes[ ]
No[x]

Test Result: Boiling Range:

5% 213 deg C
95% 216 deg C

Reference: (d) Lappin, G. [Reference 1]

C. Method other: Unknown
GLP Yes[ ]
No[x]

Test Result: 213 deg C

Reference: (b)Verschueren, [Reference 4] and (c) Weiss, [Reference]

2.3 Density:

A. Method other: Unknown
GLP Yes[ ]
No [x]

Test Results: 758 kg/m3 or 0.758 g/cm3 @ 20deg C

Reference: Verschueren, 1983 [Reference 4]

B. Method Other: ISO 3674
GLP Yes [ ]
No [ ] ?

Test Results: 0.755 – 0.765 g/cm3
Reference: (18) Shell Industrial Chemicals, Industrial Chemicals Technical Manual Higher Alpha Olefins, 1/86

C. Method other: Unknown
GLP Yes[ ]
No [x]

Test Results: 0.795 g/cm3 at 20^0C; 6.32 lb/gal at 68^0F
Reference: Lappin, G. [Reference 1]

2.4 Vapor Pressure

A. Method: Unknown
Test Value: 0.0140 kPa @ 20 deg C
0.0213 kPa @ 20 deg C

Reference: Lappin and Sauer [Reference 1]

B. Method: Unknown
Test Results: 0.159 mm Hg @ 25 deg C

Reference: Daubert and Danner, 1989

2.5 Partition Coefficient n-Octanol/water

A. Test substance: 1-dodecene
Method: calculated [X] Clog P
measured [ ]
GLP Yes [ ]
No [ ]
Test Results: log Pow = 6.1

Reference: Meylan and Howard (1995)

B. Test Substance: Shop olefin 103, C_{10-11} = 37%, C_{11-12} = 31%, C_{12} = 11%, C_{13} = 21%
Method: Calculated, Hansch and Leo (1979) primary reference

Test Results: Log P_{ow} = 5.4 – 7.0
Comments: Test report indicates a C_{10-11} =30%, but we believe the concentration to actually be 37%.
Reference: Shell, SBGR 85.182 [reference 16]

C. Test Substance: Shop olefin 103 C_{10-11} = 37%, C_{11-12} = 31%, C_{12} = 11%, C_{13} = 21%
Method: Measured
GLP Yes [X]
No [ ]

Test Results: Log Pow = >8
Comments: Test report indicates a C_{10-11} =30%, but we believe the concentration to actually be 37%.

Reference: Shell, SBGR 85.182 (Reference 16)

2.6 Water Solubility

A. Test Substance: 1-dodecene
Method:(e.g., OECD, other): Estimated in EPIWIN/ECOSAR

GLP Yes[ ]
No [x]

Test Results: Estimated 0.113 mg/L

Reference: Meylan et al., (1996); USEPA EPIWIN/ECOSAR, 99

B. Test Substance: 1-dodecene
Method: Not available
GLP Yes[ ]
No [x]

Test Results: Insoluble in water

Reference: Shell Research Report WRC 4-81 (reference 19)

C. pH/pKa- Not available

2.7 Flash Point (liquids)

A. Test Substance: 1-dodecene; C_{12} Alpha Olefin
Method (e.g., OECD, other including reference to the standard test used): Tag closed cup ISO 2719
GLP: Yes [ ]
No [x]

Test Result: 77.0°C closed cup [x] (both references via both methods)

Reference: Lappin, G [Reference 1] and Shell Specification Sheet [Reference 13]

B. Test Substance: Neodene; Alpha Olefin 12
Method: Setaflash, ASTM D-3278

Test Result: 74.8° C closed cup [x] (b)

Reference: Shell Material Safety Data Sheet [Reference 14]

2.8 Auto Flammability: No data available

2.9 Flammability (solid/gases)

Test Substance: Gulftene 12
Method (e.g., OECD, others): Not specified
GLP: Yes [ ]
No [x]

Test Results: 205 deg C

Reference: Chevron MSDS (1992)

2.10 Explosive Properties: No data available

2.11 Oxidizing Properties: No data available

2.12 Oxidation Reduction Potential: No data available

2.13 Additional Remarks:

A. Freezing point:
Test Substance: 1-dodecene
Method: Not mentioned

Test Result: -35 degree C

Reference: Weiss, G. [Reference 3]

B. Freezing Point:
Test Substance: C_{12} Alpha Olefin
Method: ISO 3013

Test Result: -36 degree C

Reference: Shell Specification Sheet [Reference 13]

C. Auto ignition temperature
Test Substance: 1-dodecene
Test Result: 225 C

Reference: Chemical Engineering [Reference 5]

D. Viscosity:

a. 1.18 cP at 20 degree °C
b. 0.741 cP at 50 degree °C

Reference Lappin, G [Reference 1]

E. Refractive index:
Test Substance: C_{12} Alpha Olefin
Method: Unknown and Shell Method Series 473

Test Results: 1.4.3 at 20 °C[ab]

Reference: Pattys [Reference 6] and Shell Specification Sheet [Reference 13]

F. Test Substance: C_{12} Alpha Olefin
Color
Pt-Co scale for clear liqids: 5 max Saybolt:
Method: ISO 2211
Reference: Shell Specification Sheet [Reference 13]

G. Reactivity and corrosive properties: Reacts when exposed to catalysts producing internal olefins and/or dimers, trimers, tetramers or high oligomers. Contact with oxygen results in slow formation of hydroperoxides which can decompose to carbonyl- containing impurities. UV-light increases the hydroperoxide formation. Hydroperoxides can interfere with reactions of 1-dodecene and cause danger of explosions.

Alpha olefins will damage many rubbers, paints and lining materials.

Reference: Lappin, G [Reference 1]

3. Environmental Fate and Pathways

3.1 Stability

3.1.1 Photo degradation
Test Substance: 1-dodecene
Method: Calculated using EPIWIN, 99, AOPWIN, input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C
Test results:
Air: cm^3/mol-sec (Half-life)
OH Rate Constant 3.3 hrs.
Overall Ozone Rate Constant 22.92 hrs

Reference: USEPA, EPIWIN, 99, model output by OPPT/RAD/ECAB Amuel Kennedy , 8/99.

3.1.2 Stability in Water: Hydrolysis: No data

3.1.3 Stability in Soil:

A. Soil Adsorption

Test Substance: 1-dodecene
Test Method or estimation method (e.g. OECD others): Estimated

GLP Yes [ ]
No [ ]

Test Results: The $C_6 - C_{12}$ alkenes are expected to volatize from the soil surface to the atmosphere. The high soil adsorption coeffecients determined for these compounds range from 3,500 to 660,000 suggesting that they will be essentially immobile in soil except when large volumes of material are present to aid in the dissolution of the alkenes (i.e. leaking underground storage tank (gasoline)). Thus, they are not expected to leach into the ground water. Strong adsorption to soil may attenuate the rate at which they volatize to the atmosphere.

Reference: jj) ITC, IR-427 Update (1990 –91)

3.2 Monitoring Data (environment)

3.3 Transport and Distribution between environmental compartments including estimate environmental concentration and distribution pathways.

3.3.1 Transport: Volatilization from water:
Test Substance: 1-dodecene
Method: Calculated using EPIWIN 99 input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Test Results:

Water: in Half-life Parameters:
Water depth 1 meter
Wind velocity 5m/sec
Current velocity 1m/sec
River Environment: 1.3 hrs
Lake Environment: 5.1 days
Pond Environment: 17 months

Reference: USEPA, EPIWIN, 99, model output by OPPT/RAD/ECAB Amuel Kennedy , 8/99. HSDB, 96

3.3.2 Theoretical Distribution (Fugacity Calculations)

A. Type of transport and distribution processes between compartments (e.g. air, water, soil):

Test substance: 1-dodecene
Results:
Level III Fugacity model:
Utilizing default values Utilizing (emission rates of 10kg/hr to air, 1 kg/hr to air, 0 kg/hr to soil as per American Chemistry Council)

Air %:	1.24	Air %:	3
Water%:	19.6	Water%:	12
Soil %:	53.4	Soil %:	<1
Sediment%:	25.8	Sediment%:	85

Summary of the method (or model) used: Calculation Method or according to Mackay, level III [1999] input values: wat sol. = 0.113; VP= 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C utilizing default emission values

Reference: USEPA/OPPT/EETD/EAB; EQC model output for 1-dodecene. David Lynch, (11/17/2000).

B. Type of transport and distribution processes between compartments (e.g. air, water, soil):

Test substance: 1-dodecene
Results:
Level I Fugacity model:

Air %:	84.9
Water%:	<1
Soil %:	14.7
Sediment%:	<1

Summary of the method (or model) used: Calculation Method or according to Mackay, level I [2000] input values: wat sol. = 0.113; VP= 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Reference: USEPA/OPPT/EETD/EAB; EQC model output for 1-dodecene. David Lynch, (11/17/2000).

3.4 Mode of Degradation in Actual Use:

Rate: Degrade fast
Reference: EPIWIN, 1999 (SRC)

3.5 Biodegradation:

A. Test substance: Shop Olefins 103 (C_{10} = 19%; C_{11} = 30%; C_{12} = 30%; C_{13} = 21%)
Test type, aerobic [x], anaerobic [ ]
Test medium:
In the case of poorly soluble chemicals, treatment given (nature, concentration, etc..):
Test method (e.g., OECD, ISO, others): Closed Bottle Test
GLP Yes [x]
No [ ]

Test Results: $C_{10} - C_{13}$ was readily biodegradable in closed bottle test with greater than 60% of the theoretical oxygen demand being consumed in 28 days

Reference: Shell Report, SBGR 85.106, [Reference 17]

B. Test substance: Shop Olefins 103 (C_{10} = 19%; C_{11} = 30%; C_{12} = 30%; C_{13} = 21%)
Test type, aerobic [x], anaerobic [ ]
Test medium:
Test method (e.g., OECD, ISO, others): Modified Sturm Test
GLP Yes [x]
No [ ]

Test Results: partially degraded in the modified sturm test with 32 to 46% of the theoretical carbon dioxide being evolved in 28 days

Reference: Shell Report, SBGR 85.106, [Reference 17]

C. Test substance: Shop Olefin 103, C_{10} = 19%, C_{11} = 30%, C_{12} = 30%, C_{13} = 21%
Test type, aerobic [x], anaerobic [ ]
Test medium: Pseudomonas fluorescens

Test method (e.g., OECD, ISO, others): Microbial Inhibition Test
GLP Yes [x]
No [ ]

Test Results: maximum inhibition of growth of 19% for concentration up to 1000 mg/L in the microbial inhibition test

Reference: Shell Report, SBGR 85.106, [Reference 17]

D. Test Substance: 1-dodecene
Test type: Aerobic
Test Method: Estimated using EPIWIN, input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Test Results: weeks (Fast)
Comments: Soil or water;

Reference: USEPA, EAB-IRER, 97; USEPA EPIWIN, 99

E. Test Substance: 1-hexadodecene

Test Results: However, JETOC, No. 5, December, 1991 list 1-hexene and 1-hexadecene among 31 readily biodegradable chemical substances as a result of testing results announced by the Japanese Ministry of International Trade and Industry (MITI) in December 1989.

Reference: JETOC, No. 5, December 1991 (Reference 28)

3.6 BOD-5, COD or Ratio BOD-5/COD: No data available

3.7 Bioaccumulation:

Test substance: 1-dodecene
Test method (e.g., OECD, other): calculated using EPIWIN, input values: wat sol. = 0.113; VP = 0.159mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Test results:
Bioaccumulation factor: 313
Calculated results: 313

Reference: USEPA, EPIWIN, 1999

3.8 Additional Remarks:

A. Sewage Treatment:

Test Substance: 1-dodecene
Test Medium: Waste Water Treatment with a rotary disk contact aerator
Test Results: 98% of 1-dodecene was eliminated with a rotating disk aerator.
Reference: CRCS, Inc. [Reference 23]

B. Test Substance: 1-dodecene
Test Medium: Secondary Wastewater Treatment (water)
Test Method: Calculated, EPIWIN, secondary wastewater treatment removal model; input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C
Test Results: 90% of 1-dodecene is eliminated with bacteria providing a minimum role in the removal process.

Comments: Both stripping to air and adsorption to sludge are expected to be important, as may biodegradation.

Reference: EPIWIN, 1999 (SRC)

C. Migration to Groundwater
Test Substance: 1-dodecene
Test Method: Calculated via EPIWIN; input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Test Results: Rate: Migration in Ground water: Slow to negligible

Reference: HSDB, 1999; EAB-IRER, 1997; EPIWIN, 99.

D. Sorption to Soil and Sediment
Test Substance: 1-dodecene
Test Method: Calculated via EPIWIN; input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Test Results: Rate: Strong Soil: K_{oc} =5864
Comments: Also considered strong in suspended organic matter in aqueous environments.

Reference: HSDB, 1996; EPIWIN, 1999 ; EAB-IRER, 97

E. Volatilization from Soil:
Test Substance: 1-dodecene
Test Method: Calculated via EPIWIN; input values: wat sol. = 0.113; VP = 0.159 mmHg; Log Kow = 6.10; BP = 168.3^{0}C; MP = -35.2^{0}C

Test Results: Rate: Dry Soil: Not expected
Moist Soil: Rapidly
Soil Mobility: Slight

Reference: HSDB, 1999; EPIWIN, 1999 ; Swann et al, 1983

4. Ecotoxicological Data

4.1 Acute/Prolonged Toxicity to fish

A. Results of acute tests

Test substance: Shop olefin 103, C_{10-11} = 30%, C_{11-12} = 31%, C_{12} = 11%, C_{13} = 21%
Test species*: Salmo gairdneri*,
Test method (e.g., OECD, others): 4-day growth test
Type of test static [x], semi-static [], flow-through [ ]
GLP Yes [x]
No [ ]

Test results:
LC50 or EC50 – values after 24, 48, 72, and 96 hours and method used to calculate these values *Salmo gairdneri* – 96-hr LC50 >1000 mg/L

Reference: Shell Report SBGR 85.182, [Reference 16]

B. Test Substance: 1-dodecene
Test Species: Fish
Test Method: Estimated via EPIWIN, 99 –Input values: Water solubility = 0.113 mg/L, VP = 0.159 mmHg, Log Kow = 6.10, BP = 168.33^{0}C, MP = -35.2^{0}C

Test Results: Test Species: fresh water fish: LC_{50} (96 hr) = 0.017 ppm

Test Species: salt water fish: LC_{50} (96 hr) = 0.029 ppm

Reference: USEPA EPIWIN, 8/99, OPPT/RAD/ECAB, run by Amuel Kennedy.

4.2 Acute Toxicity to Aquatic Invertebrates - Daphnids

A. Test substance: Shop olefin 103, C_{10-11} = 30%, C_{11-12} = 31%, C_{12} = 11%, C_{13} = 21%
Test species*: Daphnia magna*.
Test method (e.g., OECD, others): Static Water Test
GLP Yes [x]
No [ ]

Test results: 24-hr EC50 720 mg/L; 48-hr EC50 480 mg/L

Reference: Shell Report SBGR 85.182, [Reference 16]

B. Test substance: 1-dodecene
Test Species: *Daphnia magna*
Test Method: Estimated utilizing USEPA EPIWIN, 99 Input values: Water solubility = 0.113 mg/L, VP = 0.159 mmHg, Log Kow = 6.10, BP = 168.33^{0}C, MP = -35.2^{0}C

Test Results: LC_{50} (48 hr) = 0.025 ppm

Reference: USEPA EPIWIN, 8/99, OPPT/RAD/ECAB, run by Amuel Kennedy.

4.3 Toxicity to Aquatic Plants (e.g Algae)

A. Test substance: Shop olefin 103, C_{10-11} = 30%, C_{11-12} = 31%, C_{12} = 11%, C_{13} = 21%
Test species: *Selenastrum capricornutum*
Test method (e.g., OECD, others): 4 day Growth Test
GLP Yes [x]
No [ ]

Test results:
EC50 (duration, e.g. 24, 48, 72 hours)
96-hr EC50 based on cell numbers at day 4 was calculated to be 22 mg/L
Maximum concentration at which no effect was observed within the period of the test
Minimum concentration at which effect was observed within the period of the test

Reference: Shell Report SBGR 85.182, [Reference 16]

B. Test substance: 1-dodecene
Test species: Algae
Test method (e.g., OECD, others): Predicted model from ECOSAR Input values: Water solubility = 0.113 mg/L, VP = 0.159 mmHg, Log Kow = 6.10, BP = 168.33^{0}C, MP = -35.2^{0}C

Test results: EC_{50} (48 hr) = 0.020 mg/L
ChV (96-hr) = 0.021 mg/L,

Comments: ECOSAR model used to predict the chronic toxicity of 1-dodecene.

Reference: ECOSAR, 1999. Syracuse Research Inc., 1999

4.4 Toxicity to Bacteria: No data available

4.5 Chronic Toxicity to Aquatic Invertebrates:

4.5.1 Chronic Toxicity to Fish:

Test Substance: 1-dodecene
Test species: Fish
Test method (e.g., OECD, others): Predicted model from ECOSAR Input values: Water solubility = 0.113 mg/L, VP = 0.159 mmHg, Log Kow = 6.10, BP = 168.33^{0}C, MP = -35.2^{0}C

Test results: LC_{50} (14 day) = 0.061 mg/L
LC_{50} (30-day) = 0.004 mg/L

Comments: ECOSAR model used to predict the chronic toxicity of 1-dodecene.

Reference: ECOSAR, 1999. Syracuse Research Inc., 1999

4.5.2 Chronic Toxicity to Aquatic Invertebrates (Daphnia Reproduction):

Test Substance: 1-dodecene
Test Species: Daphnia
Test Method: Predicted using ECOSAR Input values: Water solubility = 0.113 mg/L, VP = 0.159 mmHg, Log Kow = 6.10, BP = 168.33^{0}C, MP = -35.2^{0}C

Test Results: EC_{50} (16 day) = 0.008 mg/L

Reference: USEPA, EPIWIN, ECOSAR, OPPT/RAD/ECAB, Amuel Kennedy, 8/99

4.6 Toxicity to Terrestrial Organisms: No data available

4.6.1 Toxicity to Soil dwelling organisms: No data available

4.6.2 Toxicity to terrestrial plants: No data available

4.6.3 Toxicity to Birds: No data available

5. Toxicological Data

5.1 Acute toxicity

5.1.1 Acute oral toxicity

A. Test Substance: Alpha Olefin 103 PQ 11,
Test Species: Rats/Wistar
GLP Yes [ ]
No [x]

Test Results: LD50 >7.7 g/kg or 7700 mg/kg

Reference: Shell Report TLGR.0171.77 [Reference 7]

B. Test Substance: C_{10} –C_{14} alpha olefin (blend not specified)
Test Species: Rats and Mice
GLP Yes [ ]
No [x]

Test Results: LD50 or other measure of acute toxicity (e.g., in case of fixed-dose text
21.3 g/kg(rat); 17.3 g/kg (Mouse)

Reference: Abasov, D. [Reference 8]

C. Test Substance: C_{12} –C_{16} alpha olefin (blend not specified)
Test Species: Rats/Wistar
GLP Yes [ ]
No [x]

Test Results: LD50 or other measure of acute toxicity (e.g., in case of fixed-dose text >10 g/kg

Reference: Rinehart, William E. [Reference 18]

D. Test Substance: C_{12} alpha olefin
Test Species: Sprague Dawley rats
GLP Yes [ ]
No [x]

Test Results: LD50 or other measure of acute toxicity (e.g., in case of fixed-dose text>10 g/kg

Reference: Ethyl Report [Reference 22]

5.1.2 Acute inhalation toxicity

A. Test substance: Olefins 103 PQ 11, AO blend of C_{10} –C_{13} (blend not specified)
Test species/strain: Rat/wistar
Test method (e.g., OECD, EC, Limit test): A group of 5 male and 5 female rats were exposed to 4 hours
GLP Yes [ ]
No [x]

Test results: (4 hr) LC50: saturated concentration (>2.1 mg/L)

Comments: Some rats lachrymated and salivated during exposure, but no other toxic signs were observed during the 14 day observation period.

Reference: Shell Report TLGR.80.052 [Reference 12]

B. Test substance: C_{10} –C_{14} alpha olefin
Test species/strain: Mouse
Test method (e.g., OECD, EC, Limit test):
GLP Yes [ ]
No [x]

Test results: LC50: saturated concentration (223.1 mg/L)

Reference: Abasov, D. [Reference 8]

C. Test substance: C_{12} –C_{16} alpha olefin
Test species/strain: Rats/Wistar
Test method (e.g., OECD, EC, Limit test):
GLP Yes [ ]
No [x

Test results: The inhalation of respirable mists less than 8 Φ of about 9900 mg/m^3 for 1 hr caused no deaths in experimental animals. A very slight “grogginess” and lethargy were the only singes of toxicity, and this disappeared rapidly when animals were removed from exposure.

Reference: Rinehart, William E. [Reference 18]

5.1.3 Acute dermal toxicity

A. Test substance: Alpha olefin 103 PQ 11
Test species/strain: Rat/Wistar
Test method (e.g., OECD, limit test):
GLP Yes [ ]
No [x]

Test results: Low order of acute dermal toxicity LD50>3.04 g/kg

Reference: Shell Report TLGR.0171.77 [Reference 7]

B. Test substance: C_{10} –C_{14} alpha olefin
Test species/strain: Rabbits
Test method (e.g., OECD, limit test):
GLP Yes [ ]
No [x]

Test results: Low order of acute dermal toxicity LD50> 10 g/kg

Reference: Rinehart, William E. [Reference 18]

C. Test substance: C_{12} –C_{16} alpha olefin
Test species/strain:
Test method (e.g., OECD, limit test):
GLP Yes [ ]
No [x]
Test results: Low order of acute dermal toxicity LD50> 10 g/kg

Reference: Ethyl Report [Reference 22]

5.2 Corrosiveness/Irritation

5.2.1 Skin Irritation

A. Test substance: Alpha olefin 103, PQ 11
Test species/strain: Rabbit/New Zealand White (8, 4M and 4F)
Method: Occlusive patch test of Draize
GLP: Yes [ ]
No [X]
Test results: A single 24h application of the test material to occluded rabbit skin was severly irritating. Abraded skin, erythema mean score: 24h=1.5, 72h=1,4, 7day=2.8; Non abraded skin, erythema mean score: 24h=1.6, 72h=1.4, 7day=2.3. Abraded skin, oedema mean score: 24h=2.3, 72h=1.3, 7day=2.3; Non abraded skin, oedema mean score: 24h=2.6, 72h=1.6, 7day=2.

Reference: Shell report TLGR.0171.77 [Reference 7

B. Test substance: Shop olefins 103, C_{10-11} = 37%; C_{11-12} = 31%; C_{13} = 21%; alpha C_{12} = 11% Test species/strain: Rabbit/New Zealand White
Method: 0.5 mL undiluted material, on application, occluded 24 hrs
GLP: Yes [X]
No [ ]

Test results: Moderate to severe irritant; 2.318 at 48 and 72 hrs; Group mean 24, 48 and 72 hrs; Erythema =1.7, Oedema=0.5

Reference: Shell Report SBGR 85.166 [Reference 9]

C. Test substance: C_{12} –C_{16} blend
Test species/strain: Rabbits
Method: 0.5 mL undiluted material, occluded 24 hrs
GLP: Yes [ ]
No [X]

Test results: Total average 0.4, slightly irritating.

Reference: Rinehart, William E, [Reference 18]

D. Test substance: Gulftene 12
Test species/strain: Rabbit/New Zealand White
Method: Draize Test (OECD 404)
GLP: Yes [X]
No [ ]

Test results: Primary irritation index of 4.67.
Mean scores of 2.2 for erythema/eschar formation and 2.4 for oedema

Comments: No corrosive effects were noted. 4 hour single dose observations at 30 min, 24, 48 and 72 hrs; 96 hrs, 7 day and 14 day indicate well defined moderate to severe erythema and slight to severe oedema which cleared by day 14.

Reference: Chevron, Gulftene 12, Acute Dermal Irritation Test in the Rabbit, SPL Project 703/078 (1996).

E. Test Substance: Alpha Olefin C_{12}
Test Species/strain: Rabbit/ New Zealand White
Method:
GLP: Yes [ ]
No [ ]

Test results: Draize score of 0.1; non-irritant

Reference: Ethyl Corporation [reference 22]

5.2.2 Eye Irritation

A. Test substance: C_{10} –C_{13} alpha olefin
Test species/strain: Rabbit/New Zealand White
Test method (e.g., OECD, others): Draize
GLP Yes [ ]
No [x]

Test results: given maximum scores after….hrs.
Practically non-irritating and non-irritating (EEC Scoring Method); mean score for conjunctional redness <0.33

Reference: Shell Report TLG.0171.77 [Reference 7]

B. Test substance: C_{10} –C_{14} alpha olefin
Test species/strain: Rabbit/New Zealand White
Test method (e.g., OECD, others): Non-Standard
GLP Yes [ ]
No [x]

Test results: Non-irritating; application of one drop to rabbit eye did not cause pathological changes

Reference: Abasov, D. [Reference 8]

C. Test substance: C_{12} –C_{16} Blend
Test species/strain: Rabbits
Test method (e.g., OECD, others): Non-Standard
GLP Yes [ ]
No [x]

Test results: Non-irritating

Reference: Rinehart, William E., [Reference 18]

D. Test substance: C_{12} alpha olefin
Test species/strain: Rabbit/New Zealand White
Test method (e.g., OECD, others):Non-Standard
GLP Yes [ ]
No [x]

Test Results: Not an eye irritant

Reference: Ethyl Report [Reference 22]

5.3 Skin sensitization

A. Test substance: C_{10} –C_{13} alpha olefin
Test species/strain: Guinea Pig/"P" Strain
Test method (e.g., OECD others): Magnusson and Kligman
GLP Yes [ ]
No [x]

Test Results: Not a skin sensitizer; no positive response were obtained in either test or control groups
Reference: Shell Report TLGR.0171.77 [Reference 7]

B. Test substance: C_{12} –C_{16} alpha olefin

Test species/strain: Guinea Pig/"P" unspecified
Test method (e.g., OECD others): Modified "Landsteiner"
GLP Yes [ ]
No [x]

Test results: Not a skin sensitizer

Reference: Rinehart, William E. [Reference 18]

5.4 Repeated dose toxicity:

A. Test substance: C_{12}- C_{16} alpha olefin blend (Gulftene 12-16)
Test species/strain: Rat/Fischer 344
Test method (e.g., OECD,other): Dermal doses of 2.0 g/kg (undiluted) or 1.0 g/kg (diluted 1:1 in corn oil) of Gulftene 12-16 were administered to groups of 5 male and 5 female rats in 9 daily doses over a 2-week period. The control group received 9 daily dermal applications of the corn oil vehicle. Approximately 6 hours following application, residual test substance was wiped from the application site. Parameters evaluated for treatment-related effects included survival, body weight, food consumption, appearenc3e and behavior, dermal reaction, hematology, clincal chemistry, organ weights, organ weight ratios relative to body weight and brain weights, gross pathology, microscopic pathology (control and high-dose animals only).
GLP Yes [X], No[]

Test Results: Repeated application of undiluted Gulftene 12-16 at 2.0 g/kg produced severe erythema (beet redness) to slight eschar formation (injuries in depth) and slight edema (edges of area well defined by definite raising) in all animals. Desquamation, hair loss and fissuring were also noted. Dermal reactions increased in severity with the numbers of applications.

When Gulftene 12-16 was administered at 1.0 g/kg, 2 animals exhibited very slight erythema (barely perceptible) after 6 treatments and a third animal after 7 treatmensts. In 1 of 3, the intensity of the erythema increased to slight and a pinpoint spot of eschar was observed after the 7^{th} treatment. All reactions persisted throughout the study period. No edema or other reactions were noted.

In comparison to controls, 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 body weights were associated with a decrease in absolute weights of most organ systems. The changes in body weights resulted in statistically significant differences in the relative and organ/brain weight ratios for several organs. No treatment related effects were noted for food consumption, clincical signs (other than dermalreactions), hematology, and clinical chemistry.. Treatment was associated with histological changes in the skin at the point of application. There were no other microscopic changes seen that could be associated with the test substances.

Under conditions of the study it was concluded that repeated dermal applications of Gulftene 12-16 at 2.0 g/kg, but not at 1.0g/kg, caused severe skin reactions and depressed body weight gains. NOAEL (systemic0 = 1g/kg/day.

Reference: Gulf Life Sciences Center (1983) Two-Week Repeated Dose Toxicity Study in Rats Using Gulftene 12-16. Conducted for Gulf Oil Chemicals Company, unpublished report.

5.5 Genetic toxicity

A. Bacterial Test

1. Test Substance: C_{11} –C_{12} alpha olefin (Blend not specified)
Test species/strain: *Salmonella typhimurium* (TA 1535, TA1537, TA1538, TA98,

TA100) and *Escherichia coli* WP_2 or WP_2 uvrA
Test method (e.g., OECD, others): Reverse mutation assay at 31.25, 62.5, 125, 250, 500, 1000, 2000, or 4000 ug per plate.
GLP Yes [ ]
No [X]

Test Results: $C_{11} - C_{12}$ alpha olefins tested in the stated Salmonella typherium strains and E coli strain both with and without the addition of rat liver microsomal fraction (S9) did not lead to an increase in the reverse mutation frequency in any of the strains. In one study with E.coli WP_2 (expt 2) there was a 2.5 fold ratio over control values at 31.25 ug per plate in the absence of s9 fraction only. This single increase was not seen in a second study (Expt. 4.) and was not considered to be a compound related effect.

With metabolic activation: no toxicity observed
Without metabolic activation: no toxicity observed

Genotoxic effects:

	+	?	-
With metabolic activation:	[ ]	[ ]	[X]
Without metabolic activation:	[ ]	[ ]	[X]

Reference: Shell Report, SBGR. 81.325 [Reference 10]

2. Test Substance: alpha - C_{12} alpha olefin
Test species/strain: *Salmonella typhimurium* (TA 1535, TA1537, TA1538, TA98, TA100) and *Escherichia coli* WP_2 or WP_2 uvrA
Test method (e.g., OECD, others): Reverse mutation assay, amounts tested 0.2, 2.0, 20, 200, and 2000 ug per plate.
GLP Yes [ ]
No [X]

Test Results: The addition of alpha - C_{12} product to agar layer cultures of bacterial tester strains, with or without the incorporation of rat liver S9 fraction, did not lead to the an increase in the reverse frequency in any of the strains.

With metabolic activation: no toxicity observed
Without metabolic activation: no toxicity observed

Genotoxic effects:

	+	?	-
With metabolic activation:	[ ]	[ ]	[X]
Without metabolic activation:	[ ]	[ ]	[X]

Reference: Shell Report, TLGR.80.074

B. Non-bacterial in vitro test

1. Test Substance: alpha C_{12} alpha olefin
Test species/strain: *Saccharomyces cerevisiae*
Test method (e.g., OECD, others):Mitotic gene conversion assay; amounts tested .01, .1, .5, 1.0, 5.0 mg/L
GLP Yes [x]
No [ ]

Test results: The addition of Alpha C_{12} product to liquid suspension cultures of S. cerevisae JD1, with or without the incorporation of rat liver S9 fraction, did not induce a consistent increase in mitotic gene conversion at either gene locus in two replicate experiments.

With metabolic activation: no toxicity observed
Without metabolic activation: no toxicity observed

Genotoxic effects:

	+	?	-
With metabolic activation:	[ ]	[ ]	[X]
Without metabolic activation:	[ ]	[ ]	[X]

Comments: The concentrations used were not reported as cytotoxic.

Reference: Shell Report, TLGR 80.074 [Reference 11]

2. Test Substance: Olefin C_{11-12} (Blend not specified)
Test species/strain: *Saccharomyces cerevisiae*
Test method (e.g., OECD, others):Mitotic gene conversion assay; amounts tested .01, .1, .5, 1.0, 5.0 mg/L
GLP Yes [x]
No [ ]

Test results: The addition of Olefin C_{11-12} to liquid suspension cultures of S. cerevisae JD1, with or without the incorporation of rat liver S9 fraction, did not induce a consistent increase in mitotic gene conversion. The increases seen were not repeatable, nor dose-related and were therefore not considered to be an effect of the compound.

With metabolic activation: no toxicity observed
Without metabolic activation: no toxicity observed

Genotoxic effects:

	+	?	-
With metabolic activation:	[ ]	[ ]	[X]
Without metabolic activation:	[ ]	[ ]	[X]

Reference: Shell Report, SBGR 81.325 [Reference 10]

3. Test substance: alpha C_{12}
Type of cell used: Rat liver RL1 cells (a) (b)
Test method (e.g., OECD, others): Rat liver chromosome aberration assay
GLP: Yes [x]
No [ ]

Test results: No toxic effects were observed in concentrations up to 500 ug/ml. A single exchange figure was observed but this occurred on one untreated control culture. Since no dose related increase in frequency of chromatid gaps, chromatid breaks or total chromatid aberrations were observed, it is concluded that alpha C_{12} product did not induce a direct cytogenetic effect in cultured RL_1 cells.

Negative

Reference: Shell Report, TLGR 80.074 [Reference 11]

4. Test substance: C_{11} –C_{12} alpha olefin
Type of cell used: Rat liver RL4 cells ; dose levels of 125, 250 and 500 ug/ml
Test method (e.g., OECD, others): Rat liver chromosome aberration assay
GLP: Yes [x]
No [ ]

Test results: Two chromosome assay's were conducted. The first assay was required to be repeated due to the small number of metaphases analyzed from the positive control slide. In the second assay, one exchange figure was found in one culture exposed to 500 ug/ml but this is not outside the range of aberrations found in untreated control cultures. Two cultures epxosred to 1 ug/ml (positive control) from which a total of 200 cells were analyzed and showed

17 chromosomal gaps, one acentric fragment and twelve exchange figures.

Although RL_4 cultures exposed to Olefin C_{11-12} at dose levels up to 500 ug/ml show some chromosomal damage, there was no dose-related incidence of chromosomal damage above the negative control values.
Lowest concentration producing cell toxicity:

Negative

Reference: Shell Report, TLGR 81.325 [Reference 10]

5. Test Substance: Gulftene 12 – 16 (Blend not specified)
Type of Cell used: Chinese Hamster Ovary
Test Method: CHO/HGPRT
GLP: Yes [ ] ?
No [ ]

Test Results: With and without enzymatic activation, the substance emulsified with F68 Pluronic^R polyol showed toxicity to CHO cells at a final concentration of 1,024 mcg/ml. There was no increase in the frequency of mutant cells after treatment with 2,048 mcg/ml.

Genotoxic effects:

With metabolic activation: Negative
Without metabolic activation: Negative

Reference: Gulf Oil Chemicals Company, "In vitro mammalian cell (CHO) Point mutation assay of gulftene C_{12} – C_{16}, "March 7, 1983 Project #82-102

6. Test Substance: Gulftene 12 –16 (Blend not specified)
Test Species/Strain: Mouse embryo cells, BALB/3T3
Test Method: Balb/3T3 Transformation
GLP: Yes [X]
No [ ]

Test Results: Immediate cytotoxicity was observed at 32 mcg/ml. Transformation was not observed at any level. Negative for transformation.

Reference: Gulf Life Sciences Center, BALB/3T3, Project #2070 [Reference 26]

7. Test Substance: Gulftene 12-16 (Blend not specified)
Test Species/Strain: Fischer 344 rat cells
Test Method: Unscheduled DNA synthesis
GLP: Yes [X]
No [ ]

Test Results: Cytotoxicity was observed initially at 256 mcg/ml. Unscheduled DNA synthesis was not observed at any level tested. The HPC/DNA repair test for Unscheduled DNA synthesis was negative.

Reference: Gulf, Hepatocyte Primary Culture, Project #2069 [Reference 27]

5.6 Non-bacterial test in vivo:

A. Test Substance: Gulftene 12 – 16 (Blend not specified)
Test Species/Strain: Crl:CD^R –1 (ICR) BR Swiss Mice

Test Method: Administered dermally to shaven backs of mice with disposable pipets at 5000 mg/kg. Other doses were varied by changing the volume administered

Test Results: All animals survived to scheduled sacrifice. There were no remarkable clinical findings. There was no significant treatment-related weight change in animals given Gulftene 12-16. There was no significant increase in micronucleated bone marrow erythrocytes or dose-related response.

Reference: Gulf, Micronucleus Test Mouse Bone Marrow, Gulftene 12-16 Administered by Dermal Application for 2 Days. Project 82-110.

5.7 Carcinogenicity: No data available

5.8 Toxicity to Reproduction: No data available

5.9 Teratogenicity/Developmental Toxicity: No data available.

5.10 Specific toxicity (Neurotoxicity, Immunotxicity etc.)

5.11 Experience with Human Exposure:

5.12 Other Studies:

Test substance: C_{12} Alpha olefins (and other alkenes)
Test species/strain:
Rat/Wistar, 4 or 5 males/group
Test method: 0.2 mL of the test material was placed in the mouth of rats anaesthetized to the point of apnea. As the animals began to breathe the nostrils were heal until the test material had been aspirated or the animal regained consciousness.

Test results: There is a significant aspiration hazard with $C_6 - C_{14}$ alkenes.

Comments: All the alkenes tested except 1-hexene were aspirated into the lungs but There was a distinct break in mortality between C14 and C16. From C8 to C14 all treated animals died within 24 hours. With C16 and C18 there was only one mortality (C18) . Lung weights were increase in alkenes treated animals compared to controls. The affected animals showed acute chemical pneumonitis.

Reference: Gerarde, H. [Reference 15]

Toxicodynamics/Toxicokinetics:

Comments: Expected metabolism of C_8, C_{10} and C_{12} n-1-olefins: Metabolism occurs in hepatic endoplasmic reticulum via initial formation of a transient epoxide. It is further metabolized to the corresponding glycol or conjugated with glutathione. The latter two metabolites are finally excreted in urine.

Reference:Maynert et al. (1970); Oesch (1973); Shell (1990); Watabe and Maynert (1968); Watabe and Yamada (1974)

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1-TETRADECENE (CAS N°: 1120-36-1)

FULL SIDS SUMMARY

ENDPOINT		SPECIES	PROTOCOL	RESULTS
PHYSICOCHEMICAL				
2.1	Melting Point	N/A	N/A	-12 ^{o}C
2.2	Boiling Point	N/A	N/A	252.1 ^{0}C at 1atm.
2.3	Density	N/A	N/A	.773 g/cm^{3}
2,4	Vapour Pressure	N/A	Measured	.015 mm Hg (0.02 hPa) at 25^{0}C
2,5	Partition Coefficient (Log K_{ow})	N/A	Calculated	log Pow = 7.08.
2.6	Water Solubility	N/A	Calculated	0.0004 mg/l at 25^{o}C
	pH	-----	-----	N/A
2.7	Flash Point		Closed Cup	107 ^{o}C (measured)
2.8	Autoflammability		Measured	239 ^{o}C
2.12	Oxidation: Reduction Potential	---	-	N/D
ENVIRONMENTAL FATE AND PATHWAYS				
3.1.1	Photodegradation	N/A	Calculated	In air $T_{1/2}$ = 9.3 hrs (hydroxyl radical) (Estd.) $T_{1/2}$ = 23 hours (ozone)
3.1.2	Volatilization from Water	-----	Estimated	$T_{1/2}$ (river) = 4.1 hr $T_{1/2}$ (pond) = 7.3 months
3.1.3	Soil Adsorption	-----	Estimated	K_{oc} = 19950
3.2	Monitoring Data	-----	-----	
3.3	Transport and Distribution		Calculated Mackay Level III Fugacity Level I	In Air 5% In Water 6% In Soil <1% In Sediment 89% In Air 95% Soil 5%
3.5	Biodegradation	(a) Sewage plant microorgs (b) Sewage plant microorgs (c)Anaerobic sludge	(a) OECD 301D (b) OECD 301B (c) ISO 11734	Aerobic: 62-64% (28 d.) 48-56% (28 d.) Anaerobic: 48% (98 d.)
3.7	Bioaccumulation	Aquatic organisms	Calculated	BCF = 1586

Unless noted, all test substances are considered to contain >90% 1-tetradecene.
N/A = not applicable, N/D = not determined; AO = Alpha olefin

ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Rainbow trout	OECD 203 ; Mortality ; semi-static	(a) EL0 (96 hr) = >1000 mg/l (WAF)
4.2	Acute Toxicity to Aquatic Invertebrates	Daphnid (*Daphnia magna*)	24 and 48 hr; immobility ; semi-static	24-hr EL0 = 1000 mg/L 48-hr EL0= 1000 mg/L
4.3	Toxicity to Aquatic Plants	Alga (*Selenastrum capricornutum*)	(a) OECD 201 ; growth static test	72-96-hr EL0 =1000 mg/l (WAF)
4.6.1	Toxicity to Micro-organisms (Bacteria)	(a) (*Pseudomonas fluorescens*) (b) Marine bacteria (13 spp)	(a) Microbial Inhibition Test (b) Microbial Inhibition Test	(a) No significant inhibition up to 1000 mg/L (b) No significant inhibition at saturation
4.6.2	Toxicity to Terrestrial Plants	-----	-----	-----
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (including Birds)	-----	-----	-----
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	(a) Rat; mouse (b) Rat	(a)Gavage (b) Gavage	(a) LD_{50} 17.3 g/kg (rat); 21.3 g/kg (mouse) (b) LD_{50} > 10 g/kg
5.1.2	Acute Inhalation Toxicity	(a) Mouse (b) Rat	(a) 1 hr exposure? (b) Described	(a) LC_{50} = 223 mg/l (b) LC_{50} >9900 mg/m^3
5.1.3	Acute Dermal Toxicity	Rabbit	(a) 24-hr occlusion (b) 24-hr occlusion	(a) LD_{50} >10 g/kg (b) LD_{50} = >10 g/kg
5.2.1	Skin Irritation	Rabbit	(a) 40 CFR 156.10 (b) Occlusion (c) 24-hr occlusion	(a) PII = 4.5 (24-hr exposure) (b) PII = 0.6: Not irritating (c) PDI = 0.0B1.2
5.2.2	Eye Irritation	Rabbit	(a) Described. C14-containing fraction. (b) Draize (c) Draize. Four C_{14}-containing AO cuts.	(a) Not irritating (b) Mean Draize = 1.0/110 at 24 hr; 0.7 at 48 hr.; 1.3/110 at 72 hr. No corneal/iris effects. (c) Draize scores = 2.1-3.0/110 at 24 hr; 0.0 by 72 hr. No corneal or iris effects.

Unless noted, all test substances are considered to contain >90% 1-tetradecene.
N/A = not applicable, N/D = not determined; AO = Alpha olefin

5.3	Skin Sensitization	Guinea Pig	Landsteiner technique. C_{12-16} AO mixture	Negative - Not a skin sensitizer
5.4	Repeated Dose Toxicity (Combined Repeat Dose and Reproduction Study)	Rat	Modified OECD 422; gavage dosing at 0, 100, 500 or 1000 mg/kg/bw daily for up to 51 days. Included MA and FOB on satellite females.	(NOAEL) = 100 mg/kg/d (systemic, satellite F); 1000 mg/kg/d (neurotoxicity M/F). Dose-related hydrocarbon nepropathy in all male treatment groups. Liver effects (M/F) at 500 and 1000 mg/kg/d.
		Rat	2-Week dermal toxicity study with C12-C16 alpha olefin blend	NOAEL (systemic) = 1 g/kg/d. Repeated dermal application at 2 g/kg caused severe skin reactions and depressed body weight gains.
5.5	Genetic Toxicity *In Vitro*			
A.	Bacterial Test: (a) Ames Test	(a) *S. typhimurium* TA98, TA100, TA1535, TA1537 and TA1538*;* *E. coli* WP2	(a) SHOP Olefin 13/14.	(a) All negative - (with and without activation)
	(b) Mitotic recombination	(b) *Saccharomyces cervisiae*	(b) SHOP Olefin 13/14.	(b) Negative - (with and without activation)
B.	Non-Bacterial Test: (a) Mammalian cell Chromosomal Abberration Assay.	(a) Rat Liver RL1 cells.	(b) SHOP Olefin 13/14.	(a) Negative- with and without activation.
	(b) HGPRT Assay	(b) CHO cells	(b) SHOP Olefin 13/14.	(b) Negative with and without activation.
	(c) Unscheduled DNA Synthesis	(c) Rat Hepatocyte Primary Culture	(c) SHOP Olefin 13/14.	(c) Negative.
	(d) Cell Transformation	(d) Balb/c-3T3 cell culture.	(d) SHOP Olefin 13/14.	(d) Negative.
5.6	Genetic Toxicity *In Vivo*: Micronucleus Assay	Mouse	Gulftene 12-16, AO mixture, C_{14} content about 20%.	Negative at doses of 1000, 2500, and 5000 mg/kg for 2 d.
5.8	Toxicity to Reproduction	Rat	Modified OECD 422; 90-day gavage dosing at 0, 100, 500 or 1000 mg/kg/bw daily for up to 51 days.	NOAEL Parental: 1000 mg/kg/day NOAEL F1 Offspring: 1000 mg/kg/day See also 5.4.
5.9	Developmental Toxicity/Teratogenicity	Rat	Modified OECD 422; 90-day gavage dosing at 0, 100, 500 or 1000 mg/kg/bw daily for up to 51 days.	NOAEL/Parental: 1000 mg/kg/day NOAEL/F1 Offspring: 1000 mg/kg/day No developmental effects seen through d. 4 of lactation.
5.1	Other:	Rat	Purity unspecified	Aspiration Hazard
5.11	Experience with Human Exposure	-----	-----	N/D

Unless noted, all test substances are considered to contain >90% 1-tetradecene.
N/A = not applicable, N/D = not determined; AO = Alpha olefin

SIDS DOSSIER
1-TETRADECENE (CAS No 1120-36-1)

SIDS PROFILE

1.1	CAS NO.	1120-36-1
1.2	CHEMICAL NAME	1-TETRADECENE
1.3	STRUCTURAL FORMULA	CH_2 =CH-$(CH_2)_{11}$-CH_3
2.0	OTHER CHEMICAL IDENTITIY INFORMATION	n-Tetradec-1-ene, Alpha Olefin C14 , Gulftene® 14, Neodene® 14, Tetradecylene; NERATEN® 14
3.0	SOURCES AND LEVELS OF EXPOSURE*	Manufactured in closed systems
3.1	PRODUCTION RANGE	1994 USA annual production - 40-50 million pounds [non-confidential business information]
3.2	CATEGORIES AND TYPE OF USE	Industrial intermediate - Main use is production of detergent alcohols. Also intermediate for amines, alkylsuccinic anhydride (ASA) monomer, chlorinated olefins, and alpha olefin sulfonate (AOS) surfactant.
4.0	ISSUES FOR DISCUSSION	Testing completed since the previous dossier indicates 1-hexene does not cause reproductive or developmental toxicity in rats at oral doses as high as 1000 mg/kg/day in an OECD guideline study. The only lesion reported was “hydrocarbon nephropathy ”only in male rats, an effect not considered relevant to human health.

SIDS SUMMARY

CAS NO: 1120-36-1 1-Tetradecene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
PHYSICAL-CHEMICAL								
2.1	Melting Point	Y	N	N	N	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapour Pressure	Y	N	N	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water Solubility	Y	N	N	N	N	Y	N
OTHER STUDIES RECEVED								
2.7	Flash Point	Y	N	N	Y	N	Y	N
2.8	Flammability	Y	N	N	Y	N	Y	N
2.3	Density	Y	N	N	Y	N	Y	N
ENVIRONMENTAL FATE/ BIODEGRADATION								
3.5	Aerobic Biodegradability	Y	Y	Y	Y	N	Y	N
3.5	Anaerbiotic Biodegr.	Y	Y	Y	N	N	Y	N
3.1.2	Hydrolysis	Y	N	N	N	Y	Y	N
3.1.1	Photodegradability	Y	N	N	N	Y	Y	N
3.3	Env. Fate/Distribution	Y	N	N	N	Y	Y	N
	Env. Concentration	N						
OTHER STUDIES RECEIVED ECOTOXICOLOGY								
4.1	Acute Toxicity Fish	Y	Y	Y	N	N	Y	N
4.2	Acute Toxicity Daphnia	Y	Y	Y	N	N	Y	N
4.3	Toxicity to Algae	Y	Y	Y	N	N	Y	N
4.4	Toxicity to Bacteria	Y	Y	N	Y	N	Y	N
4.5.2	Chronic Toxicity to							
	- Daphnia	Y	N	N	N	Y	Y	N
	- Algae	Y	N	N	N	Y	Y	N
	- Fish	Y	N	N	N	Y	Y	N
4.6.1	- Terrest. Organisms	N						
4.6.2	- Terrest. Plants	N						
4.6.3	- Avians	N						
4.6.4	Avian Reproduction	N						

CAS NO: 1120-36-1 1-Tetradecene		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQ'D
OTHER STUDIES RECEIVED TOXICOLOGY								
5.1.1	Acute Oral	Y	N	N	Y	N	Y	N
5.1.2	Acute Inhalation	Y	N	N	Y	N	Y	N
5.1.3	Acute Dermal	Y	Y	N	Y	N	Y	N
5.2.1	Corrosivity, Irritation	Y	Y	N	Y	N	Y	N
5.2.2	Eye Irritation	Y	Y	N	Y	N	Y	N
5.3	Skin Sensitization	Y	Y	N	Y	N	Y	N
5.4	Repeated Dose	Y	Y	Y	N	N	Y	N
5.5	Genetic Toxicity							
	- Gene Mutation	Y	Y	N	Y	N	Y	N
	- Chromosomal Aberrations	Y	N	N	Y	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.12	Metabolism	Y??	N	N	N	N	Y	N
OTHER STUDIES RECEIVED								
5.11	Aspiration Hazard	Y	N	N	N	N	NA	N

Summary of Responses to the OECD Request for Available Data on HPV Chemicals

REVISED: October 2000

1. General Information

1.01 Substance Information

A.	CAS No.:	1120-36-1
B.	Name (IUPAC):	Tetradec-1-ene
C.	Name (OECD)	
D.	CAS Decriptor:	
E.	EINECS-NO.:	214-306-9
F.	Molecular Formula:	$C_{14}H_{28}$
G.	Structural Formula:	CH_3-$(CH_2)_{11}$-CH=CH_2
H.	Substance Group:	Alkene
I.	Substance Remark:	
J.	Molecular Weight:	196

1.04 OECD Information

A. Sponsor country: United States

B. Lead Organization: United States Environmental Protection Agency

Contact Point:
Mr. Oscar Hernandez
US Environmental Protection Agency (USEPA)
Director, Risk Assessment Division
(USEPA/OPPTS/RAD/7403)
1201 Constitution Ave, NW
Washington, DC 20460
TELEPHONE: 1-202-564-7649
TELEFAX: 1-202-564-7450

C. Name of Responder:

American Chemistry Council (Alpha Olefins Panel)
1300 Wilson Blvd.
Alexandria, Virginia 22209, USA

Panel Manager: Doug Anderson
Telephone: (703) 741-5616
Fax: (703) 741-6091

1.1 General Substance Information

A.	Type of Substance:	Organic
B.	Physical State:	Liquid

C. Purity of industrial product: >80% w/w. Typically 94 to 96 percent pure; purity varies according to manufacturer and production process.

1.2 Synonyms: Tetradecylene, C14 Alpha Olefin, 1-Tetradecene, Alpha Tetradecene, n-Tetradec-1-ne

1.3 Impurities: Impurities at greater than 1 wt. % can include other olefins, mainly C_{12} and C_{16}; C_{14} branched isomers (mostly vinylidene), and C_{14} linear internals, with a random distribution.

1.4 Additives: Storage under nitrogen atmosphere is commonly used in order to prevent reaction with air. Antioxidants can be added.

1.5 Quantity: United States production of alpha olefins in 1993 was listed as 439,858,000 kilograms for olefins of carbon lengths C_6 to C_{10}. Production of alpha olefins in 1993 for olefins of carbon lengths greater than C_{11} was reported as 445,578,000 kilograms. (United States International Trade Commission 1994)

1.6 Labeling and Classification

EEC-labelling (recommendation)

S-phrases 26-28-62 Soap and Water

1.7 Use Pattern

Non-dispersive use: Synthesis; Lubricants and additives

Examples of use categories are dyestuffs, intermediates, solvents, adhesives, building material agents, detergents, cleaning agents, fertilizers, plastic agents, surface treatment agents, etc.

Types of uses include industrial uses as intermediates in closed systems. This chemical is mainly used for production of detergent alcohols. It is also used to produce amines (as surfactants, and other types of additives for industrial uses), alkylsuccinic anhydride (ASA) monomer, and chlorinated olefins. Tetradecene is also used in alpha olefin sulfonate(AOS) surfactant production.

2. Physicochemical Data

2.1 Melting Point: ca. –12 Degree C
Method: Other
GLP: Unknown

Reference: Lide 1991-1992; Verschueren 1983.

2.2 A. Boiling Point: ca. 232-234 degree C @ 1013 hpa (1atm)
Method: Other
GLP: Unknown

Reference: Lide 1990-1991.

B. Boiling Point: 256 degree C
Method: Other
GLP: Unknown

Reference: Verschueren 1983.

C. Boiling Point: 252.1 degree C @ 1013 hPa (1 atm)
Method: Other
GLP: Unknown

Reference: Weiss 1986.

D. Boiling Point: 245-250 degree C
Method: Other
GLP: Unkown

Comment: Boiling range is for 5% to 95%.

Reference: Lappin 1989

E. Boiling Point: 245-251 degree C
Method: ISO 4626
GLP: Unknown

Comment: C14 alpha-olefin >92.0%.

Reference: Shell 1989.

2.3 Density

A. Density: ca. 0.7745 g/cm^3 @ 20 degree C
Method: Other
GLP: Unknown

Reference: Lide 1991-1992.

B. Density: 0.76 g/cm^3 @ 20 degree C
Method: Other
GLP: Unknown

Reference: Lappin 1989

C. Density: 0.765–.775 g/cm^3 @ 20 degree C
Method: ISO 3675
GLP: Unkown

Reference: Shell 1989.

2.4 Vapor Pressure

A. Vapor Pressure 0.015 mm Hg @ 25 degree C
Method Measured
GLP No data

Reference: Daubert 1989.

B. Vapor Pressure 0.0012 hPa (0.009 mm Hg) @ 20 degree C
Method Other (calculated)
GLP No data

Reference: Lappin 1989

2.5 Partition Coefficient (Log Kow) 7.08
Method: Calculated
GLP: N/A

Reference: USEPAa 1999

2.6 Water Solubility

A. Water Solubility $4x10^{-4}$ mg/L
Method: Estimation
GLP: Unknown

Reference: USEPA 1999

B. Water Solubility Not soluble
Method: Other
GLP: Unknown

Reference: Hawley 1987.

C. Water Solubility Not soluble
Method: Other
GLP: Unknown

Reference: Lyman 1982.

2.7 Flash Point

A. Flash Point 102 degree C
Method: Other
GLP: Unknown

Reference: Shell 1989.

B. Flash Point 107.2 degree C
Method: Closed cup
GLP: Unknown

Reference: Lappin 1989

C. Flash Point 106.7 degree C
Method: Closed cup; Setaflash, ASTM D-3278.

GLP: No

Reference: Shell 1991.

D. Flash Point 102 degree C
Method: Closed cup; ISO 2719.
GLP: Unknown
Reference: Shell 1989

E. Flash Point 110 degree C
Method: Closed cup
GLP: Unknown

Reference: National Fire Protection Guide 1991

2.8 Autoflammability

A. Autoflammability 235 degree C
Method: Other
GLP: Unknown

Reference: National Fire Protection Guide 1991

B. Autoflammability 239 degree C
Method: Other
GLP: Unknown

Reference: Chemical Engineering 1972

3. Environmental Fate and Pathways

3.1 Stability

3.1.1 Photodegradation--Air

Method: Estimation
Concn. of Subst.
Temperature 25-degree C
Half-life, $t_{1/2}$ 9.3 hr (reaction with HO radical)

Comment: If released to the atmosphere, 1-tetradecene may undergo removal by gas-phase reactions with atmospheric oxidants. An estimated rate constant for the gas-phase reaction of 1-tetradecene with photochemically produced hydroxyl radicals of 4.2 x 10^{-13} cu cm/molecules-second (Atkinson 1987) translated to an atmospheric half-life of 9.3 hours using an average atmospheric hydroxyl radical concentration of 5 x 10^{5} molec/cu cm.

Reference: Atkinson 1987. Cited in the Hazardous Substance Data Bank 1995.

3.1.2 Reaction with atmospheric ozone

Method: Estimation
Concn. of Subst.
Temperature degree C
Half-life, $t_{1/2}$ 23 hr (reaction with ozone)

Comment: If released to the atmosphere, 1-tetradecene may undergo removal by gas-phase reactions with atmospheric oxidants. An estimated rate constant for the gas phase reaction of 1-tetradecene with ozone of 1.2 x 10^{-17} cu cm/molecule-second translates to an atmospheric half-life of 23 hours using an average atmospheric ozone concentration of 7 x 10^{11} molec/cu cm. (Atkinson 1987).

Reference: Atkinson 1987. Cited in the Hazardous Substance Data Bank 1995.

3.2 Transport and Distribution between Environmental Compartments

3.2.1 Transport:

A. Media: Soil/Air
Method: Estimation
Result: Immobile in soil: see comment

Comment: If released to soil, estimated soil adsorption coefficients ranging from 19,700 to 32,300 (HSDB, calculated by SRC (consultant to HSDB) using the methods of Lyman, et al., 1982, and Meylan and Howard, 1991, and the vapor pressure from Daubert, 1989) indicate that 1-tetradecene will be essentially immobile in soil (Swann 1983; USEPA, EXAMS II, 1987). Its estimated Henry's Law constant, 8.48 atm-cu m/mole (Meylan 1991), indicates that 1-tetradecene may rapidly volatilize from moist soil to the atmosphere, although expected strong adsorption to soil may attenuate the rate of this process (HSDB, calculated by SRC (consultant to HSDB) using method of Meylan and Howard, 1991). The vapor pressure of 1-tetradecene, 1.5x10^{-2} mm Hg at 25 deg C (Daubert 1989) indicates that volatilization from dry soil to the atmosphere will be very slow.

Reference: All cited in the Hazardous Substances Data Bank 1999.

B. Media: Water/Air
Method: Estimation

Half-life, $t_{1/2}$
River: 4.1 hr
Pond: 7.3 mo

Comment: Its estimated Henry's Law constant, 8.48 atm-cu m/mole (HSDB, calculated by SRC (consultant to HSDB) using the methods of Meylan and Howard, 1991), indicates that 1-tetradecene may rapidly volatilize from water to the atmosphere. The estimated half-life for volatilization from a model river 1 m deep flowing at 1 m/sec with a wind speed of 3 m/sec is 4.1 hrs (HSDB, calculated by SRC (consultant to HSDB) using method of Lyman et al.). Its expected strong adsorption to soil may attenuate the rate of this process. The estimated half-life for volatilization from a model pond, which takes into account adsorptive processes, is 7.3 months (HSDB, calculated by SRC (consultant to HSDB) using method of Swann et al., 1983).

Reference: Cited in the Hazardous Substances Data Bank 1999.

3.2.2 Distribution:

A. Type of transport and distribution processes between compartments (e.g. air, water, soil):

Test substance: 1-tetradecene
Results: Level III Fugacity model:

Utilizing Default values	Utilizing emission rates as provided by Exxon Biomedical
Air %: 1	Air %: 5
Water%: 14	Water %: 6
Soil %: 50	Soil % <1
Sediment%: 35	Sediment%: 89

Summary of the method (or model) used: Calculation Method or according to Mackay, level III [1999]; default values are 1,000 kg/hr—emission rates as provided by American Chemistry Council are: 10 kg/hr to air, 1 kg/hr to water, 0 kg/hr to soil.

Reference: USEPA/OPPT/EETD/EAB, EQC model output for 1-tetradecene. David Lynch 11/17/00.

B. Type of transport and distribution processes between compartments (e.g. air, water, soil):

Test substance: 1-tetradecene
Results:
Level 1 Fugacity model:
Air %: 94.9
Water%: <1
Soil %: 5
Sediment%: <1

Summary of the method (or model) used: Calculation Method or according to Mackay, level I [2000] input values: Utilizing default values

Reference: USEPA/OPPT/EETD/EAB, EQC model output for 1-tetradecene. David Lynch 11/17/00.

3.3 Biodegradation

A. Aerobic Based on percent of theoretical 28-d. oxygen demand.

Test substance: 1-Tetradecene, 98%
Inoculum: Prepared according to guideline

Concentration: 2 mg/L
Method: OECD Guideline 301 D
GLP: Yes

Results: Readily biodegradable: 62-65 percent after 28 days

Kinetic:
5 Day: 47-51%
15 Day: 80-87%
28 Day 62-65%

Comment: The test substance was emulsified in Dobane PT sulphonate. The apparent discrepancy between 15-day and 28-day values was explained by increased oxygen uptake in the blanks only.

Reference: Turner 1985.

B. Aerobic: Modified Sturm test

Test substance: 1-Tetradecene, 98%
Inoculum: Prepared according to guideline
Concentration: 20 mg/L
Method: OECD Guideline 301 B
GLP: Yes

Results Partially biodegradable: 48-56 percent after 28 days

Comment: The test substance was emulsified in Dobane PT sulphonate.

Reference: Turner 1985.

C. Anaerobic
Test substance: 1-Tetradecene
Inoculum: Anaerobic Sludge
Concentration: 20 mg/L
Method: ECETOC Anaerobic biodegradation (ISO 11734)
GLP: Yes

Results: Moderate ultimate degradation: ca. 48 percent after 98 days

Comment: The tetradecene used was described as the “marketed product.” The sludge inoculum originated from a secondary digester of a municipal sewage treatment plant, and was between one and four grams of dry suspended solids per liter. Test mixture volume was 500 ml in serum bottles of about 550 ml volume. Net gas production 40.5; net Dissolved Inorganic Carbon 7.8: Extent of ultimate degradation (mean value from 5 replicates) and its 95% confidence interval was 48.3 ±15.5% (98 d.).

Reference: Steber 1998.

3.4 Bioaccumulation:

BCF: Calculated. 17500-51000

Comment: Estimated bioconcentration factors indicate that 1-tetradecene could bioconcentrate in fish and aquatic organisms in the absence of metabolism. These estimates can be calculated from appropriate regression equations (HSDB, calculated by SRC (consultant to HSDB) using the methods of Lyman, et al., 1982, and Meylan and Howard, 1991 and the vapor pressure from Daubert, 1989), an estimated Henry’s Law Constant of 8.48 at-cu m/mole at 25 degrees C. (HSDB, calculated by SRC (consultant to HSDB) using method of Meylan and Howard, 1991) and an estimated octanol/water partition coefficient of 7.3 (HSDB, calculated by SRC using methods of Lyman et al., 1982) obtained from its estimated water solubility.

Reference:	Hazardous Substances Data Bank (HSDB) 1995.
BCF:	Calculated. 1586
Reference:	USEPA/OPPT/EETD/EAB, EQC model output for 1-tetradecene. David Lynch 11/17/00.

4. Ecotoxicity

4.1 Acute/Prolonged Toxicity to Fish

Test substance:	Blend of three suppliers' 1-tetradecene, 99% purity
Type:	Semistatic
Species:	Oncorhynchus mykiss
Exposure Period:	96 hour
Analyt. Monitoring:	No
Method:	OECD Guideline 203
GLP:	Yes
Test Results:	LC50 >1000 mg/L (author assigned)
	LL0 = 1000 mg/L (EPA reviewed)

Comment: Water-accommodated fractions (WAFs) were prepared by adding the appropriate amount of 1-tetradecene to dilution water on a weight-volume basis. The WAFs were mixed for 24 hour inside a covered glass vessel using a magnetic stirrer. After the mixing period, the mixture was allowed to settle for one hour before the water phase containing the WAF was siphoned off to use. Test solutions were renewed daily using freshly prepared WAFs.

The range finding test used test concentrations of WAFs from 10, 100, and 1000 mg test article per liter, and five fish per chamber. No deaths were seen during the range finding test.

A definitive limit test was then conducted using 7 fish per chamber and two replicates each in the control and treatment (WAF from 1000 mg/L) groups. No deaths or abnormal signs were noted at any time point in the control or treated groups. The 96-hour LC50 was thus greater than WAF from 1000 mg test article/liter.

LL0 = lethal loading based on the WAF testing procedure, no mortality observed at the highest loading indicated.

Reference: Drottar 1995b.

4.2 Acute Toxicity to Aquatic Invertebrates

A.

Test substance:	Blend of three suppliers' 1-tetradecene, 99% purity
Species:	Daphnia magna
Exposure Period:	48 hour
Analyt. Monitoring:	No data
Method:	OECD Guideline 202, Part 1
GLP:	YES
Test Results:	EC50 = >1000 mg/L (author assigned)
	EL0 = 1000 mg/L (EPA reviewed)

Comment: This study was a semi-static study using a water-accommodating fraction (WAF) of test article. In the range-finding test, daphnia were exposed to the WAFs prepared from 10, 100, or 1000 mg/L test article in water. No deaths occurred during the range-finding test.

The definitive limit test used a single WAF prepared from test article at 1000 mg/L and a negative control (well water). Test organisms in the control group appeared normal and healthy throughout the test. Some organisms in the treatment group appeared to be "floating" but appeared normal when re-submerged with a drop of water. All other organisms appeared normal.

Thus, the 48-hour EC50 for Daphnia magna under the conditions of this test was greater than 1000 mg/liter (WAF).

EL0 = effect loading based on the WAF testing procedure; no effect observed at the highest loading indicated.

Reference: Drottar 1995a.

B. Test substance: 1-Tetradecene (Fluka)
Species: C. marinus; P. reticulata
Exposure Period: 96 hour
Analyt. Monitoring: No data
Method
GLP:

Test Results: EC50 = >1000 mg/L

Comment: 1-Tetradecene content of test substance probably >90%. Studies conducted by TNO using marine animals did not demonstrate mortality sufficient to calculate LC50's within the 48 hr or 96 hour test periods. Test articles were prepared by stirring a large excess of compound (either 100 or 1000 mg/L) for 24 hours. Settling was allowed for 4 hours, and then the aqueous phase used for the test. Although, in addition to the named species, certain lower 1-olefins were also tested in Daphnia magna, it appears that 1-tetradecene was not.

Conclusions for the tests were that acute toxicity was not reached within the aqueous solubility of the test material.

Reference: Adema 1981-1986.

4.3 Toxicity to Aquatic Plants e.g., Algae

Test Substance: Blend of three suppliers' 1-tetradecene, 99% purity
Species: Selenastrum capricornutum
Endpoint: Growth rate
Exposure Period: 96 hours
Analyt. Monitoring: No

Method: OECD Guideline 201
GLP: Yes

Test Results: EC50 = >1000 mg/L (author assigned)

72-96 hr EL0 = 1000 mg/L (epa reviewed)

Comment: Water-accommodated fractions (WAFs) of test article were prepared by adding the appropriate amount of test article to the culture medium on a weight-volume basis. The WAFs were mixed for 24 hours inside a covered glass vessel using a magnetic stirrer. The mixture was allowed to settle for one hour after the mixing period before the water phase containing the WAF was segregated for use as test solutions.

Two range-finding tests were conducted. The first used WAFs from 10, 100 and 1000 mg/L, and the second used WAFs from 1.0, 5.0, 10, 1000, and 1000 mg/L. The second test showed less than 50% inhibition of algal biomass at each treatment level.

A definitive limit test was conducted with a single WAF (from 1000 mg/L) and a culture medium negative control. (Cell densities were used to calculated area under the growth curve values, which were subsequently used to calculate percent inhibition values relative to the control over the 96-hour exposure period. EBC 50 values (the theoretical toxicant concentrations that would produce a 50% reduction in

algal biomass) were determined for 72 and 96 hours of exposure. Both values were determined to be greater than the water accommodating fraction form 1000 mg/L.

EL0 = effect loading based on the WAF testing procedure; no effect observed at the highest loading indicated.

Reference: Thompson 1995.

4.4 Toxicity To Microorganisms e.g. Bacteria

A. Test substance: 1-Tetradecene, 98%
Species: Pseudomonas fluorescens
Exposure Period: 6 hour
Analyt. Monitoring: No data

Method: FMB SOP 021
GLP: Yes

Test Results: EC50 = >1000 mg/L

Reference: Turner 1985.

B. Test substance: 1-Tetradecene, analytical grade
Type: Aquatic
Species: Thirteen marine bacteria
Unit:
Exposure Period:
Analyt. Monitoring:

Method:
GLP

Test Results: EC50 = >saturation level

Comment: Water samples collected from Cleveland and Victoria Point on the Brisbane coast, southeastern Queensland, Australia were cultured on marine salts medium. Thirteen different marine bacteria were isolated and transferred to new media. The test articles were dissolved in ethanol and added to media. 0.1 mg of bacterial culture containing 8×10^{10} bacteria per mL was added. Absorbance at 600 nm was determined at 16 hours to assess numbers of bacteria. 1-Tetradecene was considered not toxic up to levels of 100% saturation.

Reference: Warne 1989.

C. Test substance: 1-Tetradecene, “practical grade”
Type: Other
Species: Candida sp.
Exposure Period:
Analyt. Monitoring

Method: Other
GLP: No data

Comment: Two species of Candida which can use n-alkanes above C8 for growth (C. tropicalis NCYC4 and C. 107), and Saccharomyces carlsbergensis (NCYC 530), which cannot grow on hydrocarbons, were used in this study. Organisms were grown in conical flasks at 30EC with shaking. For testing, yeasts were collected by centrifugation, and washed with buffer before use.

When tested with aliphatic compounds, glucose was at 25 g/L with 2.5 g malt extract/L of basal salts medium. This medium (20 mL) was in 100 mL flasks and inoculated with 0.1 mL of glucose-grown yeast. Alkanes and derivatives were tested at 10% (v/v). Candida

107 was grown for one day, and the other yeast grown for 3 days. A Beckman laboratory oxygen analyzer was used for respiration measurements.

Good growth was seen in all three yeast tests with tetradecene and glucose. Good growth was seen with tetradecene alone in Candida 107 and C. tropicalis. No growth was seen with Saccharomyces carlsbergensis and tetradecene in the absence of glucose.

Reference: Gill 1972.

5. Toxicity

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

A. Test substance: "C_{10} to C_{14} Alpha olefins"
Species: Mouse; rat
Method: Other
GLP: no
Value: LD50 17.3 g/kg (Mouse); 21.3 g/kg (Rat)

Comment: Test substance was an olefins fraction distilled at 180–240 deg C containing 75% monoolefin. C_{14} concentration in the test substance was not determined.

Reference: Abasov 1977.

B. Test Substances: C_{12-14} olefin, C_{14-18} olefin, C_{14-26} olefin, and C_{14-16} olefin.
Species: Rat
Method: Other
GLP: No

Test Result: LD50 = >10000 mg/kg

Comment: A large number of olefin cuts were tested for single dose acute toxicity in rats. After a fast of 18 hours, a single oral dose of 10 gram/kg of body weight was given. Survival was such that the LD50 values for all of the test articles were greater than 10 grams per kg body weight.

Reference: Gulf South Research Institute 1977

5.1.2 Acute Inhalation Toxicity

A. Test substance: C_{10} to C_{14} Alpha olefin
Species: Mouse
Exposure Time:
Method: Other
GLP: No

Test Result: LC50 = 223 mg/L.

Comment: Test substance was an olefins fraction distilled at 180–240 deg C containing 75% monoolefin. C_{14} concentration in the test substance was not determined.

Reference: Abasov 1977.

B. Test substance: C_{12} to C_{16} alpha-olefin mixture (98.5% olefin)
Species: Rat
Exposure Time: 1 hr
Method: Other
GLP: No

Test Result: LC50 = >9900 mg/L.

Comment: C_{14} concentration in the test substance was undefined; analysis of the product Gulftene 12-16 shows 16-25% C_{14} and 65-80% C_{12}. A group of ten male albino Wistar rats were exposed for one hour to saturated mists of test article. Animals were observed for 14 days after exposure. There were no deaths nor

effects on body weight during the observation period. No notable gross pathology was noted on necropsy.

The saturated mist was generated by placing a Dautrebande nebulizer in the exposure chamber and passing the air line and olefin feed line to it from outside the chamber. Particles produced by the nebulizer were no larger than 8 microns in diameter and considered respirable. Airflow of 2 liters per minute with about 50 mL of test article in the reservoir was found to produce maximum mist concentration. Estimates of mist concentration were made from loss of test material in the reservoir and the airflow through the system. Also, a sample holder containing a millipore filter was positioned downward in the chamber and air drawn at a rate calculated to collect suspended particles of 2 microns or less (the settling velocity of larger particles would have obviated capture). The lower size limit of collection by the filter was expected to be 0.45 microns. Papers were weighed before and after collection and weight gain used to calculate concentration of particles in the 0.45 to 2.0 micron range.

Estimated exposure concentration for the C_{12}-$_{16}$ olefin test article was 9900 mg/m^3 for less than 8 micron particles and 100 mg/m^3 for particles between 0.45 and 2 microns. These concentrations were very heavy mists. Visibility into the chamber was very limited.

Reference: Rinehart 1967.

5.1.3 Acute Dermal Toxicity

A. Test substance: C_{12} to C_{16} alpha-olefin mixture (98.5% olefin)
Species: Rabbit
Method: Other
GLP: No

Test Result: LD50 = >10000 mg/kg

Comment: C_{14} content of test substance unknown. A single group of 4 male albino rabbits were used. The hairs over the back were clipped on all animals, and two of the four then were abraded over the test site. Ten grams of test article per kilogram of body weight was applied to the test site, and gauze pads and an impervious wrap were applied over the sites. Test article remained in contact with the skin for 24 hours. Animals were observed for 14 days. One rabbit died of pneumonia in that period. The death was not considered test article related.

Reference: Rinehart 1967.

B. Test Substance: C_{12-14} olefin, C_{14-18} olefin, C_{14-26} olefin, and C_{14-16} olefin.
Species: Rabbit
Method: Other
GLP: No

Test Result: LD50 = >10000 mg/kg

Comment: A large number of olefin cuts were tested for single dose dermal toxicity in rabbits. Six New Zealand white rabbits (male and female) were used per test article. A dose of 10 grams per kilogram body weight was applied to clipped and abraded test sites. Sites were occluded for 24 hours and animals observed for 14 days. Survival was such that LD50's were stated to be greater than 10 grams per kilogram body weight.

Reference: Gulf South Research Institute 1977

5.2 Corrosiveness/Irritation

5.2.1 Skin Irritation

A. Test substance: C_{14} alpha olefin, “Neodene 14"
Species: Rabbit
Method: 40 CFR 156.10
GLP: Yes

Test Result: Primary irritation index = 4.5 (severely irritating).
Classification: Irritating

Comment: C_{14} content of test substance 95%. A group of three male and three female New Zealand rabbits was used in this patch test. Primary irritation index was reported as 4.5, “severely irritating.”

Reference: Morris 1992

B. Test substance: C_{12} to C_{16} alpha-olefin mixture (98.5% olefin)
Species: Other
GLP: No

Test Result: Not Irritating
Classification: Not Irritating

Comment: C_{14} content of test substance unknown. A group of six albino rabbits were used in this patch test for irritation. Backs were clipped of hair and intact and abraded sites were prepared. One-half milliliter of test article was applied to two intact and two abraded sites per animal. The test sites were covered with gauze pads and tape. No further wrappings were used as the test articles either evaporated or were absorbed quickly. Skin reaction were noted after 24 and 72 hours.

No edema was noted at any time point. Mean erythema scores for the 24 and 72 hour readings were 0.8 and 0.2 for the intact and 1.2 and 0.2 for the abraded sites. Maximum individual score was a “2” in one animal at intact and abraded sites at 24 hours only. Average Primary Irritation Score was 0.6.

Reference: Rinehart 1967

C. Test Substances: C_{12-14} olefin, C_{14-18} olefin, C_{14-26} olefin, and C_{14-16} olefin.
Species: Rabbit
Method: Other
GLP: No

Test Result: Not Irritating
Classification: Not Irritating

Comment: Olefins cuts were tested for single dose dermal irritation. Six New Zealand white rabbits (male and female) were used per test article. A dose of 0.5 mL of test article was applied to intact and abraded test sites. Sites were occluded for 24 hours and observations for redness and edema were made at 24 and 72 hours. Primary dermal index scores (out of a possible total of 8.0) were 0.0 (C_{14-26}; C_{12-14}), 0.14 (C_{14-18}) and 1.2 (C_{14-16}).

Reference: Gulf South Research Institute 1977

5.2.2 Eye Irritation

A. Test substance: See Comment
Species: Rabbit
Method: Other
GLP: No

Test Result: Not Irritating
Classification: Not Irritating

Comment: Test substance was an olefins fraction distilled at 180–240 deg C containing 75% monoolefin. C_{14} concentration in the test substance was not determined. Application of one drop to rabbit eyes did not cause pathological changes.

Reference: Abasov 1977.

B. Test substance: C_{12} to C_{16} alpha-olefin mixture (98.5% olefin)
Species: Rabbit
Method: Draize test
GLP: No

Test Result: Not Irritating
Classification: Not Irritating

Comment: C_{14} content of test substance unknown. Groups of six male albino rabbits were used. A positive control group was exposed to 5% Ivory Soap solution; other groups received olefin test article. A single dose of 0.1 mL of undiluted test article was placed in one eye. Exposed eyes were not washed out, and observations were made at 24, 48, and 72 hours.

No scores greater than zero were seen in any animal for the cornea or iris at any time point. Maximum erythema scores were “1” in three of the six animals at 24 hours. Two animals had a score of “1” for erythema at 48 hours; four animals had “1” at 72 hours. Draize score at 24 hours was 1.0/110; it was 0.7 at 48 hour and 1.3 at 72 hours.

Reference: Rinehart 1967

C. Test Substances: C_{12-14} olefin, C_{14-18} olefin, C_{14-26} olefin, and C_{14-16} olefin.
Species: Rabbit
Dose: 0.1 mL
Method: Draize test
GLP: No

Test Result: Not irritating
Classification: Not Irritating

Comment: Olefin cuts were tested for single dose ocular irritation in rabbits. Six New Zealand white rabbits (male and female) were used per test article. A dose of 0.1 mL was applied to one eye. Observations for redness and edema of the conjunctiva, and the appearance of the iris and cornea were made at 24,48, and 72 hours. Draize scores (out of a possible total of 110.0) were 3.0 (C12-14), 2.7 (C14-26; C14-18) and 2.1 (C14-16) at 24 hours. All scores were 0.0 by 72 hours. No corneal or iris effects were seen.

Reference: Gulf South Research Institute 1977

5.3 Skin Sensitization

A. Test substance: C_{12} to C_{16} alpha-olefin mixture (98.5% olefin)
Type: Landsteiner technique
Species: Guinea Pig
Method: Other
GLP: No

Test Result: Not sensitizing
Classification: Not Sensitizing

Comment: C_{14} content of test substance unknown. Groups of ten male albino guinea pigs were used. A positive control group was exposed to 0.5% chlorodinitrobenzene in 50%

ethyl alcohol. A second group was exposed to 50% ethyl alcohol only. The other group received olefin test article. Test sites on the backs of the animals were clipped, and scored with a needle. One-tenth mL of the test article was applied by glass rod to the test sites three times weekly for nine applications. Observation for erythema and edema were made 24 hours after application. After the ninth application, animals were rested for two weeks. They were then challenged with 0.1 mL of test article.

Only slight erythema was seen in on or two of the animals exposed to the alpha olefin after the eight applications. No edema was seen. Animals exposed to alcohol only showed no reaction at any time point. The positive control animals showed moderated redness after the third application, and mild edema in half the animals.

At the challenge, alpha-olefin-exposed animals showed no response. The positive control group showed increased response to chlorodinitrobenzene.

Conclusion was that animals treated with C_{12-16} olefin were not sensitized within the limits of this test.

Reference: Rinehart 1967

5.4 Repeated Dose Toxicity

A. Test substance:	Blend of three suppliers' 1-tetradecene, 99% purity
Species:	Rat
Strain:	Sprague-Dawley
Sex:	Male/Female
Route of Admin.:	Gavage
Exposure Period:	Up to 51 days; see Comment
Freq. of Treatment:	Once Daily
Post-Exposure:	Observ. Period
Doses:	0, 100, 500, or 1000 mg/kg/day
Control Group:	Concurrent vehicle
Method:	Modified OECD 422
GLP:	Yes
Test Result:	
NOAEL	100 mg/kg/day (systemic) 1000 mg/kg/day (neurotoxicity)

Comment: This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Spraque Dawley rats. The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating, during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating and during mating, gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred. **(See sections 5.8 and 5.9 for Reproductive and Developmental Effects)**

Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day. Animals were observed daily for signs of toxicity, and body weights and food consumption were measured at intervals. Breeding females were allowed to deliver and raise offspring until lactation day 4. All F0 males and females were subjected to gross necropsy when euthanized. Selected F0 males and all satellite females were evaluated for motor activity, clinical pathology, and functional observational battery before euthanasia. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, on selected tissues from five randomly selected males and females from the control and high dose groups, and on the lungs, liver, kidneys, and reproductive tracts of all females.

Minor clinical signs (salivation and urine staining) were noted in satellite females and F0 parent animals. Dose-related hydrocarbon nephropathy was noted in kidneys of male rats in all groups. Male and female rat livers showed hepatocyte cytoplasmic vacuolation to some degree in the 500 and 1000 mg/kg/day groups. This was associated with increases in liver weights. There were no test article-related differences in the functional observational battery and motor activity tests that would indicate neurotoxicity. The NOAEL for neurotoxicity was 1000 mg/kg/day in males and females. For systemic effects, the NOAEL was 100 mg/kg/day in the satellite females. Since hydrocarbon nephropathy was seen in all male dose groups, there was not a NOAEL for male rats for systemic toxicity. However, male rat hydrocarbon nephrophathy is unique to the male rat, and does not suggest an adverse effect for human risk assessment.

Reference: Daniel 1995

B. **Test substance: C_{12}- C_{16} alpha olefin blend (Gulftene 12-16)**
Test species/strain: Rat/Fischer 344
Test method (e.g., OECD,other): Dermal doses of 2.0 g/kg (undiluted) or 1.0 g/kg (diluted 1:1 in corn oil) of Gulftene 12-16 were administered to groups of 5 male and 5 female rats in 9 daily doses over a 2-week period. The control group received 9 daily dermal applications of the corn oil vehicle. Approximately 6 hours following application, residual test substance was wiped from the application site. Parameters evaluated for treatment-related effects included survival, body weight, food consumption, appearenc3e and behavior, dermal reaction, hematology, clincal chemistry, organ weights, organ weight ratios relative to body weight and brain weights, gross pathology, microscopic pathology (control and high-dose animals only).
GLP Yes [X], No[]

Test Results: Repeated application of undiluted Gulftene 12-16 at 2.0 g/kg produced severe erythema (beet redness) to slight eschar formation (injuries in depth) and slight edema (edges of area well defined by definite raising) in all animals. Desquamation, hair loss and fissuring were also noted. Dermal reactions increased in severity with the numbers of applications.

When Gulftene 12-16 was administered at 1.0 g/kg, 2 animals exhibited very slight erythema (barely perceptible) after 6 treatments and a third animal after 7 treatments. In 1 of 3, the intensity of the erythema increased to slight and a pinpoint spot of eschar was observed after the 7^{th} treatment. All reactions persisted throughout the study period. No edema or other reactions were noted.

In comparison to controls, 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 body weights were associated with a decrease in absolute weights of most organ systems. The changes in body weights resulted in statistically significant differences in the relative and organ/brain weight ratios for several organs. No treatment related effects were noted for food consumption, clinical signs (other than dermal reactions), hematology, and clinical chemistry.. Treatment was associated with histological changes in the skin at the point of application. There were no other microscopic changes seen that could be associated with the test substances.

Under conditions of the study it was concluded that repeated dermal applications of Gulftene 12-16 at 2.0 g/kg, but not at 1.0g/kg, caused severe skin reactions and depressed body weight gains. NOAEL (systemic0 = 1g/kg/day.

Reference: Gulf Life Sciences Center (1983) Two-Week Repeated Dose Toxicity Study in Rats Using Gulftene 12-16. Conducted for Gulf Oil Chemicals Company, unpublished report.

5.5 Genetic Toxicity in vitro

A. Bacterial Reverse Mutation Assay

Test substance: "SHOP Olefin C13/14"; not further characterized.
Test species: Salm. Typhimurium and E. coli strains

Concentration:
Metabolic Activation: With and without
Method: Other
GLP: Yes

Test Result: Negative

Comment: There was no consistent increase in reverse mutation rate in the bacterial tester strains with or without S9. The concentrations tested were not reported to be cytotoxic.

Reference: Brooks 1982.

B. Mitotic recombination

Test substance: “SHOP Olefin C13/14"; not further characterized.
Species: Saccharomyces cervisiae
Concentration:
Metabolic Activation:
Method: Other
GLP: Yes

Test Result: Negative

Comment: There was no increase in mitotic gene conversion in Saccharomyces cervisiae.

Reference: Brooks 1982.

C. Mammalian cell gene mutation assay

Test substance: “SHOP Olefin C13/14"; not further characterized.
Test system: Rat Liver RL1 cells
Concentraion:
Metabolic Activation: With and Without
Method: Other
GLP: No data

Test Result: Negative

Comment: Test article did not increase the incidence of chromosome aberrations in rat liver cells in vitro. There was no cytotoxicity.

Reference: Brooks 1982.

D. HGPRT assay

Test substance: Gulftene 12-16, olefin mixture, C_{12} to C_{16}.
Test system: Chinese Hamster Ovary Cell
Concentration: 128, 512, 1024, and 2048 ug/mL
Metabolic Activation: With and without
Method: Other
GLP: Yes

Test Result: Negative

Comment: C_{14} concentration in the test substance was undefined; analysis of other Gulftene 12-16s shows 16-25% C_{14} and 65-80% C_{12}. Test article was emulsified with F68 Pluronic polyol. Activating Enzymes were S9 derived from rats treated with Aroclor 1254. Test system was Chinese Hamster Ovary cells (CHO-K1) obtained from Dr. J.P. O’Neill of Oak Ridge National Laboratories.

In range-finding tests, some toxicity was evident at 2,048 ug/mL without activation; and with 64 to 2048 ug/mL with activation. Toxicity was within acceptable limits.

In the definitive test, a toxic effect was noted in that there were insufficient cells to subculture at 1 X 10^6 per dish at the 1024 and 2048 levels without activation and that cultures with activation also showed immediate toxicity at those levels. Colony counts after subculture showed that cells which were used to determine the mutagenic effect were able to grow and had recovered from the initial toxic effect. The frequency of mutant colonies was increased to expected values in the two positive control groups indicating the assay was functional. There were no increases over control in frequency of mutant colonies when cultures were treated with test article.

Reference: Gulf Life Science Center 1983c

E.Unscheduled DNA Synthesis

Test substance: Gulftene 12-16, olefin mixture, C_{12} to C_{16}.
Test system: Rat Hepatocyte Primary Culture
Concentration: 100 ug/mg, 1000 ug/mL, 2000 ug/mL, and 4000 ug/mL
Metabolic Activation:
Method:
GLP: Yes

Test Result: Negative

Comment: C_{14} concentration in the test substance was undefined; analysis of other Gulftene 12-16s shows 16-25% C_{14} and 65-80% C_{12}. F68 Pluronic polyol was the vehicle control. 2-Acetylaminofluorene (AAF, 0.2 ug/mL) was the positive control. Tritiated thymidine was the radionuclide used. Primary hepatocytes derived from freshly perfused F344 rat liver were used. Williams Medium E was supplemented with 10% fetal bovine serum and insulin, and antibiotics were included. Final concentrations used in the UDS portion of the study were 100, 1000, 2000, and 4000 ug/mL. Three cultures were used for each level of test substance and positive and negative control substances. Cultures were seeded with about 1 x 10^5 cells per mL on day 1, and then exposed for 18 hour to the radionuclide and test substance. Cells growing on cover slips were rinsed, exposed to hypotonic solution, fixed, air dried and glued to microscope slides on day 2. On day 3 the slides were dipped in autoradiographic emulsion and stored in the dark at 2-8 degrees C until developed and stained on day 13.

The numbers of grains overlying each of 50 randomly selected nuclei per slide were counted.

The highest of 3 cytoplasmic grain counts per cell was subtracted to obtain the net nuclear grain count. Both the positive and negative controls gave expected results. No treatment level of Gulftene 12-16 gave a positive response (no treatment level gave a mean net nuclear count greater than 6 grain per nucleus over the negative control; and the negative control did not exceed 5).

Reference: Gulf Life Science Center 1984

F.Cell Transformation

Test substance: Gulftene 12-16, olefin mixture, C_{12} to C_{16}.
System of Testing: BALB 3T3-A31-1-1 Mouse Embryo Cells
Concentration: 10 ug/mL, 20 ug/mL, 30 ug/mL, and 1500 ug/mL
Metabolic Activation:
Method: Other
GLP: Yes

Test result: Negative

Comment: Test article (C_{14} concentration undefined; analysis of other Gulftene 12-16s shows 16-25% C_{14} and 65-80% C_{12}) was emulsified with F68 Pluronic polyol. Cells were obtained from Dr. T. Kakunaga, National Cancer Institute. Positive control was 3-methylcholanthrene (final concentration of 1 ug/mL). Vehicle control was F68 Pluronic polyol. Cells were grown in Eagle's Minimum Essential Medium supplemented with 10% heat-inactivated fetal calf serum.

In range-finding cytotoxicity tests, toxicity was evident at 32 ug/mL with 16% relative viability following a 2-day exposure period. Viability remained near this level up to a dose of 2048 ug/mL. At 5000 ug/mL, viability was reduced to 1.3%.

In the definitive test, a toxic effect was noted at 20 ug/mL Gulftene 12-16 (27% relative cloning efficiency) and remained at this level through the highest concentration tested (1500 ug/mL). The positive control gave the expected response for the transformation. The negative controls were within acceptable limits for the test. No treatment level exceeded the system (medium) control for type III foci.

Reference: Gulf Life Sciences Center 1983b

5.6 Genetic Toxicity in Vivo: Micronucleus Assay

Test substance: Gulftene 12-16, olefin mixture, C_{12} to C_{16}.
Species: Mouse
Sex: Male/Female
Strain: Swiss
Route of Admin: Dermal
Exposure Period: Days 1 and 2
Doses: 1000, 2500, and 5000 mg/kg/ body weight
Method: Other
GLP: No data

Test Result: Negative

Comment: C_{14} concentration in the test substance was undefined; analysis of other Gulftene 12-16s shows 16-25% C_{14} and 65-80% C_{12}. Test article was emulsified with corn oil. Negative control in the test was corn oil: cyclophosphamide was positive control. Test article was applied at a maximum volume of 0.2 mg on the shaved backs of the mice of Days 1 and 2. Cyclophosphamide was given by intraperitoneal injection at a dose of 75 mg/kg. Cyclophosphamide-treated animals were sacrificed on day 3; other groups were sacrificed and bone marrow smears prepared on days 3 and 4.

All animals (5 per sex per group) survived to sacrifice. There were no remarkable clinical findings, or effects on body weight changes. Slides from animals given corn oil and cyclophosphamide gave expected results. Slides from animals give Gulftene C12-16 gave no significant increase (T-test, $p< 0.05$) in micronucleated bone marrow erythrocytes or dose related response.

Reference: Gulf Life Sciences Center 1983a

5.7 Carcinogenicity

Comment: No long-term carcinogenicity tests have been conducted on long-chain alpha olefins. However, there are no structural indicators to suggest carcinogenicity. For analogy, long-term carcinogenicity studies have been conducted for alpha olefin sulfonates (AOS) derived from alpha olefins of similar alkyl length. For example, Hunter and Benson (1976) fed rats mixed C_{14}-$_{16}$ AOS at dietary levels of 1000, 2500, and 5000 ppm for two years. Blood chemistries, urinalyses, and histopathological findings were comparable to control values. There was no increase in tumors from the feeding of the test article. Three carcinogenicity studies of AOS reported by Oba and Takei (1992) indicated that these AOS were not carcinogenic by oral or dermal routes.

Reference: Hunter 1976; Oba 1992

5.8 Toxicity to Reproduction

Test substance: Blend of three suppliers' 1-tetradecene, 99% purity
Species: Rat
Strain: Sprague-Dawley
Sex: Male/Female
Route of Admin: Gavage
Exposure Period: Up to 51 d.; see Comment
Freq. of Treatment: Daily
Premating Exposure Period
Male: Four weeks
Female: Two weeks
Duration of Test: Through Lactation day 4 for pups
Doses: 0, 100, 500, 1000 mg/kg/day
Control Group: Concurrent vehicle
Method: Other: Modified OECD 422
GLP: Yes

Test Result:
NOAEL Parental: 1000 mg/kg/day
NOAEL F1 Offspring: 1000 mg/kg/day
NOAEL F2 offspring: N/A

Comment: This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Spraque Dawley rats. The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating, during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating and during mating, gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred. **(See section 5.4--Repeated dose toxicity-- for systemic and neurotoxicity results)**

Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day. Animals were observed daily for signs of toxicity, and body weights and food consumption were measured at intervals. Breeding females were allowed to deliver and raise offspring until lactation day 4. Viability and development of the F1 generation were evaluated, and surviving F1 pups were euthanized on lactation day 4. All F0 males and females were subjected to gross necropsy when euthanized. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, on selected tissues from five randomly selected males and females from the control and high dose groups, and on the lungs, liver, kidneys, and reproductive tracts of all females.

Minor clinical signs (salivation and urine staining) were noted in satellite females and F0 parent animals. There were no differences in measurements of fertility or reproductive capacity in the F0 generation, nor were there developmental effects in the F1 generation through day 4 of lactation. The NOAEL for reproductive effects was 1000 mg/kg/day in males and females.

Reference: Daniel 1995

5.9 Developmental Toxicity /Teratogenicity

Test substance: Blend of three suppliers' 1-tetradecene, 99% purity
Species: Rat

Strain: Sprague-Dawley
Sex: Male/Female
Rout of Admin: Gavage
Exposure Period: Up to 51 d.; see Comment
Freq. of Treatment: Daily
Duration of Test: Through lactation day 4 for pups
Doses: 0, 100, 500, 1000 mg/kg/day
Control Group: Concurrent vehicle
Method: Modified OECD 422
GLP: Yes

Test Result:
NOAEL: Maternal Toxicity 1000 mg/kg/day
NOAEL: Teratogenicity 1000 mg/kg/day

Comment: This study was conducted to provide screening information on the potential for systemic, reproductive, developmental and neurotoxicity of 1-tetradecene when given orally, by gavage, to parental male and female Spraque Dawley rats. The study consisted of one control group and three treatment groups with 12 males and 20 females in each group. F0 males were treated for 28 days prior to mating, during mating and until the day prior to euthanasia (43-47 days). The twelve F0 females were dosed 14 days prior to mating, during mating gestation and lactation until the day prior to euthanasia (42-51 days). The eight remaining females per group were a satellite group for evaluation of neurotoxicity, clinical pathology and histopathology parallel to the breeding males, but were not bred. **(See section 5.4--Repeated dose toxicity--for systemic and neurotoxicity results; and section 5.8--Toxicity to Reproduction–for reproductive toxicity results.)**

Doses used in the study were 0 mg/kg/day (corn oil vehicle only), 100 mg/kg/day, 500 mg/kg/day, and 1000 mg/kg/day. Animals were observed daily for signs of toxicity and body weights and food consumption were measured at intervals. Breeding females were allowed to deliver and raise offspring until lactation day 4. Viability and development of the F1 generation were evaluated, and surviving F1 pups were euthanized on lactation day 4. All F0 males and females were subjected to gross necropsy when euthanized. Specified tissues were retained and preserved on selected males and all females. Microscopic examination was conducted on gross lesions from all animals, selected tissues from five randomly selected males and females from the control and high dose groups, and the lungs, liver, kidneys, and reproductive tracts of all females.

Minor clinical signs (salivation and urine staining) were noted in satellite females and F0 parent animals. Male and female rat livers showed hepatocyte cytoplasmic vacuolation to some degree in the 500 and 1000 mg/kg/day groups. This was associated with increases in liver weights. There were no developmental effects in the F1 generation through day 4 of lactation. The NOAEL for developmental effects was 1000 mg/kg/day in males and females.

Reference: Daniel 1995

5.10 Other Relevant Information:

Aspiration hazard assessment

Test substance: 1-Tetradecene
Species: Rat
Strain: Wistar
Sex: Male
Rout of Admin: Aspiration
Dose: 1 mL
GLP: No

Test Result: See comments

Comment: 1-Tetradecene (and other alkenes), source and purity unspecified, was assessed for aspiration hazard in an animal study using Wistar rats. Four or five males were used per test article. Two-tenths mL of the test material was placed in the mouth of rats that had been anesthetized to the point of apnea. As the animals began to breathe again, the nostrils were held until the test material had been aspirated or the animal gained consciousness. All alkenes tested except hexene were aspirated into the lungs. All animals exposed to C_8 to C_{14} died within 24 hours. With C_{16} and C_{18}, there was only one death (C_{18}). Lung weights were increased in alkenes-treated animals compared with controls. The affected animals showed chemical pneumonitis. The report concluded that there is a significant aspiration hazard with C_6 to C_{14} alkenes.

Reference: Gerarde 1963

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