SIDS INITIAL ASSESSMENT PROFILE

CAS Nos.	25264-93-1 25339-56-4 25377-83-7 27215-95-8 25339-53-1 25378-22-7 85535-87-1 629-73-2 112-88-9
Chemical Names	[in the same order shown above for CAS Nos.] hexene heptene octene nonene decene dodecene alkenes, C10-13 1-hexadecene 1-octadecene
Structural Formula	[in the same order shown above for CAS Nos.] CH_3-CH=CH-$(CH_2)_2$-CH_3[a] CH_3-CH=CH-$(CH_2)_3$-CH_3[a] CH_3-CH=CH-$(CH_2)_4$-CH_3[a] CH_3-CH=CH-$(CH_2)_5$-CH_3[a] CH_3-CH=CH-$(CH_2)_6$-CH_3[a] CH_3-CH=CH-$(CH_2)_8$-CH_3[a] CH_3-CH=CH-$(CH_2)_x$-CH_3[a] (x = 6-9) CH_3-$(CH_2)_{13}$-CH=CH_3 CH_3-$(CH_2)_{15}$-CH=CH_3 [a] Basic structure; position of internal double bond varies and some isomers may be branched

SUMMARY CONCLUSIONS OF THE SIAR

Category/Analogue Rationale

This profile includes an evaluation of SIDS-level testing data, using a category approach, with six individual internal olefins (C_6 – C_{10} and C_{12}), a C_{10-13} internal olefins blend and two linear alpha olefins (1-hexadecene and 1-octadecene), all of which are mono-olefins. The internal olefins are predominantly linear, but may contain small amounts of branched materials. For the purposes of the OECD HPV Chemicals Programme, the category was defined as "Higher Olefins." The category designation was based on the belief that internalizing the location of the carbon-carbon double bond, increasing the length of the carbon chain, and/or changing the carbon skeleton's structure from

linear to branched does not change the toxicity profile, or changes the profile in a consistent pattern from lower to higher carbon numbers. While the category is actually defined as $C_6 - C_{18}$ mono-olefins (sponsored chemicals), we included surrogate data from a mixed stream containing C_{20}-C_{24} linear and branched internal olefins. While we realize that sufficient data exist to support the category without the data on the C_{20}-C_{24}, we believe these data provide additional support and strengthen the hypothesis that changing carbon number, location of the double bond or addition of branching does not alter the mammalian health and biodegradation endpoints and helps to indicate increasing or decreasing trends for ecotoxicity data.

Human Health

Olefins (alkenes) ranging in carbon number from C_6 to C_{24}, alpha (linear) and internal (linear and branched) demonstrate low acute toxicity by the oral, inhalation and dermal routes of exposure: Rat oral LD_{50} >5 g/kg; rat 4-hr inhalation LC_{50} range = 110 mg/L (32,000 ppm) to 6.4 mg/L (693 ppm) for C_6 to C_{16}; and rat/rabbit dermal LD_{50} > highest doses tested (1.43 - 10 g/kg).

Repeated-dose studies, using the inhalation (C_6 alpha), dermal (C_{12}-C_{16}), or oral (C_6 alpha and internal linear/branched; C_8 and C_{14} alpha; and C_{16}, C_{18} and C_{20}-C_{24} internal linear/branched) routes of exposure, have shown comparable levels of low toxicity in rats. In females, alterations in body and organ weights, changes in certain clinical chemistry/hematology values, and liver effects were noted (NOELs of $\geq$ 100 mg/kg oral or $\geq$ 3.44 mg/L (1000 ppm) inhalation). In males, alterations in organ weights, changes in certain clinical chemistry/hematology values, liver effects, and male rat-specific kidney damage that is likely associated with the alpha $_{2\mu}$- globulin protein were noted (LOELs $\geq$ 100 mg/kg oral only). The male rat kidney damage was seen in oral studies with C_6, C_8 and C_{14} linear alpha olefins and C_6 internal branched olefins, but was not seen in studies with C_{16}/C_{18} or C_{20} - C_{24} internal linear/branched olefins. The noted liver effects were seen in oral studies with C_{14} alpha olefins (minimal-to-mild hepatocyte cytoplasmic vacuolation with increased liver weight in males and females) and with C_{20}-C_{24} internal olefins (minimal centrilobular hepatocyte hypertrophy with increased liver weight in females only). No effects were present in the study with C_{20}-C_{24} internal olefins following a 4-week recovery period, indicating reversibility of the observed effects. These liver effects seen only with the larger molecules may be indirect effects of an intensified liver burden, rather than a direct toxic effect of the olefin. Based on evidence from neurotoxicity screens included in repeated dose studies with C_6 and C_{14} alpha olefins and with C_6, C_{16}/C_{18} and C_{20}-C_{24} internal linear/branched olefins, the category members are not neurotoxic.

Based on evidence from reproductive/developmental toxicity screens in rats with C_6 and C_{14} alpha olefins and C_6 and C_{18} linear/branched internal olefins, along with the findings of no biologically significant effects on male or female reproductive organs in repeated dose toxicity studies, the category members are not expected to cause reproductive or developmental toxicity.

Based on the weight of evidence from studies with alpha and internal olefins, category members are not genotoxic. No carcinogenicity tests have been conducted on $C_6 - C_{18}$ alpha or internal olefins; however, there are no structural alerts indicating a potential for carcinogenicity in humans.

These materials are not eye irritants or skin sensitizers. Prolonged exposure of the skin for many hours may cause skin irritation. The weight of evidence indicates alpha and internal olefins with carbon numbers between C_6 and C_{24} have a similar and low level of mammalian toxicity, and the toxicity profile is not affected by changes in the location of the double bond or the addition of branching to the structure.

Environment

The potential for exposure of aquatic organisms to members of the Higher Olefins Category will be influenced by their physico-chemical properties. The predicted or measured water solubilities of these olefins range from 50 mg/L at 20°C for hexene to 0.00015 mg/L at 25°C for 1-octadecene, which suggests there is a lower potential for the larger olefins to be bioavailable to aquatic organisms due to their low solubilities. Their vapor pressures range from 230.6 hPa at 25°C for hexene to 0.00009 hPa at 25°C for 1-octadecene, which suggests the shorter chain olefins will tend to partition to the air at a significant rate and not remain in the other environmental compartments for long periods of

time; while the longer chain olefins will tend to partition primarily to water, soil or sediment, depending on water solubility and sorption behaviour. The soil adsorption coefficients (K_{oc}) range from 149 for C_6 to 230,800 for C_{18}, indicating increasing partitioning to soil/sediment with increasing carbon number. Level I fugacity modeling predicts that the C_6-C_{13} olefins would partition primarily to air, while the C_{16}-C_{18} olefins would partition primarily to soil. Results of Level III fugacity modelling suggest that the $C_6 – C_8$ category members will partition primarily to the water compartment; and, as the chain length increases beyond C_{10}, soil and sediment become the primary compartments. These chemicals have a very low potential to hydrolyze and do not photodegrade directly. However, in the air, all members of the category are subject to atmospheric oxidation from hydroxyl radical attack, with calculated degradation half-lives of 1.8 to 4.1 hours. $C_6 – C_{18}$ olefins have been shown to degrade to an extent of approximately 8-81% in standard 28-day biodegradation tests. These results were not clearly correlated with carbon number or any other identifiable parameter; however, the weight of evidence shows that the members of the Higher Olefins Category have potential for degradation in the environment. Volatilization from water is predicted to occur rapidly (hours to days), with Henry's Law Constants (bond method) ranging from 0.423 (C_6) to 10.7 (C_{18}) atm m^3/mol. Consideration of these degradation processes supports the assessment that these substances will degrade relatively rapidly in the environment and not persist. Based on calculated bioconcentration factors, the C_6, C_7, C_{16} and C_{18} category members are not expected to bioaccumulate (BCF = 46, 236, 71 and 3). Although the $C_8 – C_{13}$ olefins have BCFs ranging from 659 to 748, and K_{ow} values ranging from 4.13 to 6.59, and thus are considered to have the potential for bioaccumulation, their physico-chemical properties and fate indicate that there would be limited environmental exposure because of volatility, biodegradability and limited solubility.

Data indicate that acute aquatic toxicity can be observed for C_6 through the C_{10} olefins (C_6: EC/LC_{50} range of 1-10 mg/L; C_7-C_{10}: EC/LC_{50} range of 0.1-1.0 mg/L), and that toxicity increases with increasing carbon number within that range, which is consistent with increasing K_{ow} values (3.07 – 5.07). Above a chain length of 10, toxicity is not observed within the limits of solubility. However, data indicate that chronic aquatic toxicity can be observed in the C_{10} olefins (EC_{10} = 20.0 μg/L, EC_{50} = 28.1 μg/L, NOEC = 19.04 μg/L). Data also suggest that aquatic toxicity does not differ with bond location or presence of branching.

Exposure

The following U.S. production volumes for 2002 were reported for members of the Higher Olefins Category: 1-10 million pounds for hexene and dodecene, 10-50 million pounds for decene and C_{10}-C_{13} alkenes, 50-100 million pounds for heptene and octene, and 100-200 million pounds for 1-hexadecene and 1-octadecene. Members of the Higher Olefins Category are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals (including polymers, fatty acids, mercaptans, plasticizer alcohols, detergents, surfactants, additives for lubricants, amine oxides and amines, detergent alcohols and nonionics, and hydraulic fluids and additives). C_{16} and C_{18} olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. Non-occupational human exposure is not expected. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. Results from modeled data suggest that on-site waste treatment processes are expected to remove these compounds from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge. The olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

The chemicals in this category are currently of low priority for further work. These chemicals possess properties indicating hazards to human health (reversible mild skin and eye irritation; mild respiratory tract irritation to the lower chain length members) and the environment (acute aquatic toxicity for the C6-C10 category members and chronic aquatic toxicity for C10). Based on exposure data presented by the sponsor country, (four manufacturing sites within the sponsor country which accounts for 47-64% of global production depending on category member) and relating to use pattern in the sponsor country (industrial intermediate in closed systems) this category is a low priority for further work. Countries may wish to investigate any exposure scenarios that were not presented by the sponsor country.