SIDS INITIAL ASSESSMENT PROFILE

Chemical Category Name	Alkyl Sulfates, Alkane Sulfonates and α-Olefin Sulfonates
CAS No. / Chemical Name	**Alkyl Sulfates:**
	139-96-8 Sulfuric acid, mono-dodecyl ester, compound with triethanolamine (1:1) (C_{12} ASO_4 TEA)
	142-31-4 Sulfuric acid, mono-octyl ester, sodium salt (C_8 ASO_4 Na)
	142-87-0 Sulfuric acid, mono-decyl ester, sodium salt (C_{10} ASO_4 Na)
	151-21-3 Sulfuric acid, mono-dodecyl ester, sodium salt (C_{12} ASO_4 Na)
	1072-15-7 n-Nonylsulfate, sodium salt (C_9 ASO_4 Na)
	1120-01-0 Sulfuric acid, mono-hexadecyl ester, sodium salt (C_{16} ASO_4 Na)
	1120-04-3 Sulfuric acid, mono-octadecyl ester, sodium salt (C_{18} ASO_4 Na)
	1191-50-0 Sulfuric acid, mono-tetradecyl ester, sodium salt (C_{14} ASO_4 Na)
	2235-54-3 Sulfuric acid, mono-dodecyl ester, ammonium salt (C_{12} ASO_4 NH_4)
	3026-63-9 1-Tridecanol, hydrogen sulfate, sodium salt (C_{13} ASO_4 Na)
	4706-78-9 Potassium dodecyl sulphate (C_{12} ASO_4 K)
	7065-13-6 Potassium hexadecyl sulphate (C_{16} ASO_4 K)
	7739-63-1 Potassium decyl sulphate (C_{10} ASO_4 K)
	13393-71-0 Sulfuric acid, mono-pentadecyl ester, sodium salt (C_{15} ASO_4 Na)
	39943-70-9 Sulfuric acid, monodecyl ester, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (C_{10} ASO_4 TEA)
	68081-96-9 Sulfuric acids, mono-C_{10-16}-alkyl esters, ammonium salts (C_{10-16} ASO_4 NH_4)
	68081-97-0 Sulfuric acids, mono-C_{10-16}-alkyl esters, magnesium salts (C_{10-16} ASO_4 Mg)
	68081-98-1 Sulfuric acids, mono-C_{14-18}-alkyl esters, sodium salts (C_{14-18} ASO_4 Na)
	68585-47-7 Sulfuric acid, mono-C_{10-16}-alkyl esters, sodium salts (C_{10-16} ASO_4 Na)
	68611-55-2 Sulfuric acid, mono-C_{10-16}-alkyl esters (C_{10-16} ASO_4)
	68890-70-0 Sulfuric acids, mono-C_{12-15}-alkyl esters, sodium salts (C_{12-15} ASO_4 Na)
	68955-19-1 Sulfuric acids, mono-C_{12-18}-alkyl esters, sodium salts (C_{12-18} ASO_4 Na)
	68955-20-4 Sulfuric acids, mono-C_{16-18}-alkyl esters, sodium salts (C_{16-18} ASO_4 Na)
	73296-89-6 Sulfuric acids, mono-C_{12-16}-alkyl esters, sodium salts (C_{12-16} ASO_4 Na)
	85665-45-8 Sulfuric acids, mono-C_{8-14}-alkyl esters, compounds with triethanolamine (C_{8-14} ASO_4 TEA)
	85586-07-8 Sulfuric acids, mono-C_{12-14}-alkyl esters, sodium salts

		(C_{12-14} ASO_4 Na)
	85681-68-1	Sulfuric acid, mono-(C_{14-18} and C_{16-18} −unsatd.alkyl) esters, sodium salts (C_{14-18} and C_{16-18}= ASO_4 Na)
	86014-79-1	Sulfuric acid, mono-C_{13-15}-alkyl esters, sodium salts (C_{13-15} ASO_4 Na)
	90583-10-1	Sulfuric acid, mono-C_{8-14}-alkyl esters, ammonium salts (C_{8-14} ASO_4 NH_4)
	90583-12-3	**Sulfuric acids, mono-C_{12-16}-alkyl esters, ammonium salts (C_{12-16} ASO_4 NH_4)**
	90583-13-4	Sulfuric acid, mono-C_{12-18}-alkyl esters, ammonium salts (C_{12-18} ASO_4 NH_4)
	90583-16-7	Sulfuric acid, mono-C_{12-14}-alkyl esters, compounds with ethanolamine (C_{12-14} ASO_4 MEA)
	90583-18-9	**Sulfuric acids, mono-C_{12-14}-alkyl esters, compounds with triethanolamine (C_{12-14} ASO_4 TEA)**
	90583-19-0	Sulfuric acid, mono-C_{8-14}-alkyl esters, lithium salts (C_{8-14} ASO_4 Li)
	90583-23-6	Sulfuric acids, mono-C_{12-14}-alkyl esters, magnesium salts (C_{12-14} ASO_4 Mg)
	90583-24-7	**Sulfuric acids, mono-C_{12-18} alkyl esters, potassium salts (C_{12-18} ASO_4 K)**
	90583-27-0	Sulfuric acids, mono-C_{8-16}-alkyl esters, sodium salts (C_{8-16} ASO_4 Na)
	90583-31-6	Sulfuric acids, mono-(C_{14-18} and $C_{18\text{-unsaturated}}$)-alkyl esters, sodium salts (C_{14-18} and $C_{18=}$ ASO_4 Na)
	91648-54-3	Sulfuric acids, mono-C_{14-15}-alkyl esters, sodium salts (C_{14-15} ASO_4 Na)
	91783-22-1	Sulfuric acids, mono-C_{12-13}-alkyl esters, potassium salts (C_{12-13} ASO_4 K)
	91783-23-2	Sulfuric acids, mono-C_{12-13}-alkyl esters, sodium salts (C_{12-13} ASO_4 Na)
	96690-75-4	Sulfuric acid, mono-C_{12-14}-alkyl esters, ammonium salts, compds. with triethanolamine (C_{12-14} ASO_4 TEA)
	117875-77-1	**Sulfuric acids, mono-C_{10-16}-alkyl esters, compounds with triethanolamine (C_{10-16} ASO_4 TEA)**
		Sulfuric acids, mono-C_{15-16}-alkyl esters (C_{15-16} ASO_4)*
		Sulfuric acids, mono-C_{12-18}-alkyl esters, magnesium salts (C_{12-18} ASO_4 Mg)*
		Potassium undecyl sulphate (C_{11} ASO_4 K)*
	<u>Alkane Sulfonates:</u>	
	2386-53-0	Sodium dodecane-1-sulfonate (C_{12} ASO_3 Na)
	5324-84-5	**1-Octanesulfonic acid, sodium salt (C_8 ASO_3 Na)**
	13419-61-9	Sodium decane-1-sulfonate (C_{10} ASO_3 Na)
	13893-34-0	Sodium octadecane-1-sulfonate (C_{18} ASO_3 Na)
	27175-91-3	Sodium tetradecane-1-sulfonate (C_{14} ASO_3 Na)
	68815-15-6	Sulfonic acids, C_{15-18}-alkane, sodium salts (C_{15-18} ASO_3 Na)
	<u>α-Olefin Sulfonates:</u>	
	11067-19-9	Sodium hexadecene-1-sulfonate (C_{16}=/$OHASO_3$ Na)

	30965-85-6 Dodecene-1-sulfonic acid, sodium salt (C_{12} =/$OHASO_3$ Na) **68439-57-6 Sulfonic acids, C_{14-16}-alkane hydroxy and C_{14-16}-alkene, sodium salts (C_{14-16} =/$OHASO_3$ Na)** **93686-14-7 Sulfonic acids, C_{14}-alkane hydroxy and C_{14}-alkene, sodium salts (C_{14} =/$OHASO_3$ Na)** 85536-12-5 Sulfonic acids, C_{12-14}-alkane hydroxy and C_{12-14}-alkene, sodium salts (C_{12-14} =/$OHASO_3$ Na) **863609-89-6 Sulfonic acids, C_{14-18}-alkane hydroxy and C_{14-18}-alkene, sodium salts (C_{14-18} =/$OHASO_3$ Na)** 91082-14-3 Sulfonic acids, C_{15-18}-alkane hydroxy and C_{15-18}-alkene, sodium salts (C_{15-18} =/$OHASO_3$ Na) 91722-28-0 Sulfonic acids, C_{16-18}-alkane hydroxy and C_{16-18}-alkene, sodium salts (C_{16-18} =/$OHASO_3$ Na) Sulfonic acids, $C_{14/16/18}$-alkane hydroxy and $C_{14/16/18}$-alkene, sodium salts (1:1:1) ($C_{14/16/18}$ =/$OHASO_3$ Mg)* **Bold: HPV chemicals** *CAS number not available
Structural Formula	**<u>Alkyl Sulfates (AS)</u>**: **R-OSO_3^-** cation$^+$ where R = predominantly linear alkyl group of chain length C8 – C18 **<u>Primary Alkane Sulfonates (PAS):</u>** **R-SO_3^-** cation$^+$ where R = predominantly linear alkyl group of chain length C8 – C18 **<u>α-Olefin Sulfonates (AOS):</u>** **R'-CH(OH)-$(CH_2)_m$-SO_3^- Na^+** where m = 2 or 3 and **R'-CH=CH-$(CH_2)_n$-SO_3^- Na^+** where R' = alkyl group and n = 1 - 3 total alkyl chain length: C12 – C18

SUMMARY CONCLUSION OF THE SIAR

Category Justification

This category consists of three structurally related classes of anionic surfactants: alkyl sulfates with a predominantly linear alkyl chain length of C_8-C_{18}, C_8-C_{18} alkane sulfonates, and alpha-olefin sulfonates with linear aliphatic chains of typically C_{14}-C_{18}. Most chemicals of this category are not defined substances, but mixtures of homologues with different alkyl chain lengths. Alpha-olefin sulfonates are mixtures of alkene sulfonate and hydroxyl alkane sulfonates with the sulfonate group in the terminal position and the double bond, or hydroxyl group, located at a position in the vicinity of the sulfonate group.

The surfactants of this category are produced and transported as either pure solids or as aqueous solutions with typically between 30 and 95 % of active substance. Twenty-one (21) of the chemicals included in this category have HPV status in one or more OECD regions. In addition, data from 40 non HPV-chemicals were used for read-across

between the three sub-groups and the category as a whole.

The most important common structural feature of the category members is the presence of a predominantly linear aliphatic hydrocarbon chain with a polar sulfate or sulfonate group, neutralized with a counter ion (i.e., Na^+, K^+, NH_4^+, or an alkanolamine cation).

The hydrophobic hydrocarbon chain (with a length between C_8 and C_{18}) and the polar sulfate or sulfonate groups confer surfactant properties and enable the commercial use of these substances as anionic surfactants. The close structural similarities result in physico-chemical properties and environmental fate characteristic which follow a regular pattern. Common physical and/or biological pathways result in structurally similar breakdown products, and are, together with the surfactant properties, responsible for similar environmental behavior and essentially identical hazard profiles with regard to human health. The structural similarities result in the same mode of ecotoxic action. Within each subcategory the most important parameter influencing ecotoxicity is the varying length of the alkyl chain. Although the counter ion may also influence the physico-chemical behaviour of these chemicals, the chemical reactivity and classification for the purpose of this assessment is not expected to be affected by the difference in counter ion.

Human Health

Alkyl Sulfates, alkane sulfonates and α-olefin sulfonates are well absorbed after ingestion; penetration through the skin is however poor. After absorption, these chemicals are distributed mainly to the liver. Alkyl sulfates, alkane sulfonates and most probably also α-olefin sulfonates are metabolized by cytochrome P450-dependent ω-oxidation and subsequent ß-oxidation of the aliphatic fatty acids. End products of the oxidation are a C_4 sulfate or sulfonate (even numbered chain lengths) and a C_3 or C_5 sulfate or sulfonate (odd numbered chain lengths). For the alkyl sulfates in addition sulfate is formed as a metabolite. The metabolites are rapidly excreted in the urine.

Acute dermal LD_{50} values in rabbits were 200 mg a.i. (active ingredients)/kg bw for the C_{12}- and greater than 500 mg a.i./kg bw for the C_{12-13}- and C_{10-16}- alkyl sulfates, respectively; apart from moderate to severe skin irritation, clinical signs included tremor, tonic-clonic convulsions, respiratory failure, and body weight loss in the study with the C_{12}-alkyl sulfate and decreased body weights after administration of the C_{10-16}- alkyl sulfates. No data are available for alkane sulfonates but due to a comparable metabolism and effect concentrations in long-term studies effect concentrations are expected to be in the same range as found for alkyl sulfates. No specific systemic toxicity occurred in acute dermal toxicity studies with the α-olefin sulfonate C_{14-16}=/$OHASO_3$ Na on rats or rabbits at the highest tested dose level (740 mg a.i./kg bw in rats, 2325 mg a.i./kg bw in rabbits).

Acute oral LD_{50} values in rats and/or mice of alkyl sulfates were between 290 and 580 mg a.i./kg bw for C_{10}, between 1000 and 2000 mg a.i./kg bw for C_{10-16}, and C_{12}, greater than 2000 mg a.i./kg bw for $C_{12-14,}$ C_{12-15}, C_{12-16}, C_{12-18} and C_{16-18}, and greater than 5000 mg a.i./kg bw for C_{14-18} and $_{16-18}$= alkyl sulfates. The counter ion does not appear to influence the toxicity in a substantial way. The clinical signs observed were non-specific (piloerection, lethargy, decreased motor activity and respiratory rate, diarrhea). At necropsy the major findings were irritation of the gastrointestinal tract and anemia of inner organs. The LD_{50} in rats of the C_8 alkane sulfonate (sodium salt) was >5000 mg a.i./kg bw with no clinical signs of intoxication and no adverse findings at necropsy reported. LD_{50} values in rats for the C_{14-16}-α-olefin sulfonates (sodium salts) were between 578 and 2200 mg a.i./kg bw. Based on limited data, the acute oral LD_{50} values of alkane sulfonates and α-olefin sulfonates of comparable chain lengths are assumed to be in the same range.

There are no data available for acute inhalation toxicity of alkyl sulfates, alkane sulfonates or α-olefin sulfonates.

In skin irritation tests performed on rabbits in accordance with OECD TG 404, the ca. 30% aqueous solutions of C_{8-14}- and C_{8-16}, the 90% solution of C_{12-14}-, and the 60% solution of $C_{14-18/18=}$- alkyl sulfates were all corrosive. At 25%, and under occlusive conditions, C_{12}- and C_{12-14}- and at ≥ 5-7% C_{12}-, C_{12-15}-, C_{13-15}- and C_{15-16} −alkyl sulfates were moderate to strong irritants. C_{16-18} ASO_4 Na showed only slight irritation up to concentrations of 31.5%. The α-olefin sulfonate C_{14-16} =/$OHASO_3$ Na was irritating when tested at a concentration of 40% according to OECD TG 404. 5 % of an α-olefin sulfonate (C_{14-18} =/$OHASO_3$Na) were only very slightly irritating. Comparative studies investigating skin effects like transepidermal water loss, epidermal electrical conductance, skin swelling, extraction of amino acids and proteins or development of erythema in human volunteers consistently showed a maximum of effects with C_{12} ASO_4Na. 20% C_{12} ASO_4Na is routinely used as a positive internal control giving borderline irritant reactions in skin irritation studies performed on humans. With C_{12} ASO_4Na being the most irritant alkyl sulfate it can be concluded that in humans 20% is the threshold concentration for irritative effects of alkyl sulfates in general. When formulated in consumer products, alkyl sulfates are usually used in conjunction with other surfactants. These mixed surfactant

systems form micelles that typically lead to a reduction in irritation potential of the mixture, compared to the irritation potential of the individual ingredients. No data were available with regard to the skin irritation potential of alkane sulfonates. Based on the similar chemical structure they are assumed to exhibit similar skin irritation properties as alkyl sulfates or α-olefin sulfonates of comparable chain lengths.

C_{12}-containing alkyl sulfates (at concentrations ≥ 10%) were severely irritating to the eyes of rabbits and caused irreversible corneal effects. With increasing alkyl chain length, the irritating potential decreases, and $C_{16-18}ASO_4Na$, at a concentration of 25%, was only a mild irritant. Concentrated C_{14-16}- α-olefin sulfonates were severely irritating, but caused irreversible effects only if applied as undiluted powder. At concentrations below 10 % mild to moderate, reversible effects were found. No data were available for alkane sulfonates.

Alkyl sulfates and C_{14-18} α-olefin sulfonates were not skin sensitizers in animal studies performed according to OECD TG 406. In humans, the sensitizing potential of $C_{12}ASO_4$ Na is very low and C_{14-16} α-olefin sulfonate was not found to have any sensitising potential. No reliable data were available for alkane sulfonates. Based on the similar chemical structure, no sensitization is expected.

For repeated dermal application a "No Observed Adverse Effect Level" (NOAEL) of 400 mg a.i./kg bw/day for systemic effects was found in mice treated twice weekly for 3 or 13 weeks with 0.2 ml of C_{12-15} ASO_4 Na at concentrations of 0, 5, 10, 12.5 or 15% in water (corresponding to ca. 0, 200, 400, 500, or 600 mg a.i./kg bw/day). At 10% concentration, epidermal hyperplasia, and at concentrations of ≥ 12.5% in addition epidermal cytotoxicity (ulceration) was found. Increased water intake and elevated liver, kidney and heart weights were associated with concentrations >10%.

After repeated oral application of alkyl sulfates with chain lengths between C_{12} and C_{18}, the liver was the only target organ for systemic toxicity. Adverse effects on this organ included an increase in liver weight, enlargement of liver cells, and elevated levels of liver enzymes. The "Lowest observed adverse effect level" (LOAEL) for liver toxicity (parenchymal hypertrophy and increase in relative liver weight) was found for C_{16-18} ASO_4 Na in a 13-week dietary study on rats at 230 mg a.i./kg bw/day. The lowest NOAEL in rats was at 55 mg a.i./kg bw/day in a 13-week study with C_{12} ASO_4 Na.

NOAELs of about 100 mg a.i./kg bw/day were found for rats in comprehensive oral 6 month- and 2-year studies with C_{14}– and C_{14-16}- α-olefin sulfonates. At 200-250 mg a.i./kg bw/day, a reduction in body weight gain was the only adverse effect in these studies.

No data were available with regard to the repeated dose toxicity of alkane sulfonates. Based on the similarity of metabolic pathways between alkane sulfonates, alkyl sulfates and α-olefin sulfonates, the repeated dose toxicity of alkane sulfonates is expected to be similar with NOAEL and LOAEL values in the same range as for alkyl sulfates and α-olefin sulfonates, i.e. 100 and 200-250 mg a.i./kg bw/day, respectively, with the liver as potential target organ.

Alkyl sulfates of different chain lengths and with different counter ions were not mutagenic in standard bacterial and mammalian cell systems (only Na salts were tested in the latter) both in the absence and in the presence of metabolic activation. There was also no indication for a genotoxic potential of alkyl sulfates in various *in vivo* studies on mice (micronucleus assay, chromosome aberration test, and dominant lethal assay).

α-Olefin sulfonates were not mutagenic in the Ames test, and did not induce chromosome aberrations *in vitro*. No genotoxicity data were available for alkane sulfonates. Based on the overall negative results in the genotoxicity assays with alkyl sulfates and α-olefin sulfonates, the absence of structural elements indicating mutagenicity, and the overall database on different types of sulfonates, which were all tested negative in mutagenicity assays, a genotoxic potential of alkane sulfonates is not expected

Alkyl sulfates were not carcinogenic in good quality feeding studies with male and female Wistar rats fed diets with C_{12-15} ASO_4 Na for two years (corresponding to doses of up to 1125 mg /kg bw/day). No carcinogenicity studies were available for the alkane sulfonates.

α-Olefin sulfonates were not carcinogenic in mice and rats after dermal application, and in rats after oral exposure. Dermal applications in mice were carried out 3 times weekly for 92 weeks with a volume of 0.02 ml of either C_{14-16} − or C_{14-18} α-olefin sulfonates at concentrations of 20 or 25%. Rats were treated twice weekly for 104 weeks with a 10% solution of C_{14-16} =/$OHASO_3$ Na. In the oral study, Sprague-Dawley rats were dosed with up to 259 mg C_{14-16} =/$OHASO_3$ Na/kg bw/day

No fertility studies were performed with alkyl sulfates and alkane sulfonates. Oral dosing of male mice with C_{12} ASO_4

Na (1 % over 2 or 0.1 % over 6 weeks) caused no adverse effects on epididymal spermatozoa, and a NOAEL for male fertility was derived at 1000 mg a.i./kg bw/day in an earlier SIDS document for sodium dodecyl sulfate. No indication for adverse effects on reproductive organs was found in various oral studies with different alkyl sulfates. For the α-olefin sulfonates a modern two generation reproductive toxicity study in male and female CD rats was performed with a mixture of C_{14}:C_{16}:C_{18} blend (1:1:1 ratio) of α-olefin sulfonate, Mg salt. Two batches with an active ingredient content of ca. 95 % were used and the animals were continuously dosed with 0, 1250, 2500 or 5000 ppm (corresponding to about 1040 mg a.i./kg bw/day) in the diet with a protocol comparable to OECD TG 416. The animals showed no adverse effects up to and including the highest test concentration of 5000 ppm.

The developmental toxicity of various alkyl sulfates (C_{12} ASO_4 Na, C_{12-14} ASO_4 Na, C_{12-15} ASO_4, C_{13-15} ASO_4 Na, C_{15-16} AS Na, C_{16-18} ASO_4 Na) was tested on rats, rabbits and mice. Effects on litter parameters were restricted to doses that caused significant maternal toxicity (anorexia, weight loss, and death at doses between 300 and 500 mg a.i./kg bw for rats and at 300 mg a.i./kg bw/day for mice and rabbits), the principal effects being higher fetal loss and increased incidences of total litter losses. The incidences of malformations and visceral and skeletal anomalies were unaffected apart from a higher incidence of delayed ossification or skeletal variation in mice at $\geq$ 500 mg a.i./kg bw/day indicative of a delayed development. The lowest reliable NOAEL for maternal toxicity was about 200 mg a.i./kg bw/day in rats, while the lowest NOAELs in offspring were 250 mg a.i./kg bw/day in rats and 300 mg a.i./kg bw/day for mice and rabbits.

For the α-olefin sulfonates no adverse effects were reported in rats (dams and offspring) dosed with up to 600 mg a.i./kg bw/day of C_{14-16} =/$OHASO_3$ Na during days 6-15 of pregnancy, i.e. the NOAEL was 600 mg a.i./kg bw/day both for maternal and developmental toxicity. From a parallel study with mice and rabbits no clear NOAEL can be derived due to an unusual spreading of the applied doses (0, 0.2, 2, 300 and 600 mg a.i./kg bw/day). At 2 mg a.i./kg bw/day no adverse effects were found, while at 300 mg a.i./kg bw/day adverse effects both in dams and offspring were observed.

No data were available for the reproductive and developmental toxicity of alkane sulfonates. Based on the available data, the similar toxicokinetic properties and a comparable metabolism of the alkyl sulfates and alkane sulfonates, alkane sulfonates are not considered to be developmental toxicants.

Although the database for category members with C<12 is limited, the available data are indicating no risk as the substances have comparable toxicokinetic properties and metabolic pathways. In addition, longer-term studies gave no indication for adverse effects on reproductive organs with different alkyl sulfates.

Environment

For sodium salts of alkyl sulfates, measured melting points are in the range of 181 °C (C_8) to 193 °C (C_{16}). Calculated melting points are in the range of 232 °C (C_8) to 286 °C (C_{16}).

Measured melting points for alkane sulfonates, alkene sulfonates, and hydroxy alkane sulfonates are not available. Calculated melting points are in the ranges of 227 - 281 °C (C_{8-18} alkane sulfonates), 250 - 283 °C (C_{12-18} alkene sulfonates) and 274 - 296 °C (C_{14-18} hydroxy alkane sulfonates).

As ionic substances, all members of this category have extremely low vapor pressures. Calculated values are in the ranges 10^{-11} to 10^{-15} hPa (C_{8-18} alkyl sulfates), $4.3 \cdot 10^{-11}$ to $9 \cdot 10^{-15}$ hPa (C_{8-18} alkane sulfonates), $2.1 \cdot 10^{-13}$ to $6.9 \cdot 10^{-15}$ hPa (C_{14-18} alkene sulfonates) and $3.3 \cdot 10^{-17}$ to $5.8 \cdot 10^{-19}$ hPa (C_{14-18} hydroxy alkane sulfonates). Therefore, they decompose before reaching their theoretical boiling points.

Measured water solubilities are available only for alkyl sulfates; they are in the range 196 000 mg/l (C_{12}) to 300 mg/l (C_{16}) and by factors of 50 to 300 higher than calculated values (C_{12}: 617 mg/l, C_{16}: 5 mg/l).

As surfactants have a tendency to concentrate at hydrophilic/hydrophobic boundaries rather than to equilibrate between phases K_{OW} is not a good descriptor of surfactant hydrophobicity and only of limited predictive value for the partitioning of these compounds in the environment.

All calculated physico-chemical properties of surfactants should be treated with caution, because the estimation models do not take into account surfactant properties. In addition, the results are doubtful for ionic substances.

Deduced from physico-chemical and surfactancy properties the target compartment for the substances of this category is the hydrosphere. Based on the ionic structure partitioning into the atmosphere can be excluded. In water, the

compounds are stable to hydrolysis under environmental conditions.

Taking into account the low BCF factors (≤ 73) up to C_{16} that were determined for alkyl sulfates, any significant bioaccumulation is not expected.

Soil sorption increases with chain length. Strong sorption on soils would be expected for chain length 14 upwards. Sediment concentrations were between 0.0035 and 0.021 mg/kg dw indicating that accumulation in sediments is low. Under certain conditions of reduced moisture in soil, i.e. in arid or semi-arid regions, accumulation in soil cannot be excluded.

The substances of this category are readily biodegradable. Significant biodegradation of alkyl sulfates in the raw sewage, i.e. in the sewer system before reaching the WWTPs is very likely. The substances of this category are quantitatively removed in WWTP's, mainly by biodegradation. Because of the anaerobic degradation of alkyl sulfates in sewage sludge, exposure of agricultural soils due to application of sludge as fertilizer is not expected. However, for alkane sulfonates and α-olefin sulfonates this exposure pathway cannot be excluded due to their recalcitrant or limited anaerobic degradability.

The aquatic toxicity is influenced by a number of parameters, the length of the alkyl chain being most important. The pH and temperature of water bodies can affect the EC/LC_{50} values for compounds that contain ammonium ions.

The most sensitive trophic level in tests on the toxicity of **alkyl sulfates** were invertebrates, followed by fish. Algae proved to be less sensitive. The key study for the aquatic hazard assessment is a chronic test on *Ceriodaphnia dubia*, which covers a range of the alkyl chain length from C_{12} to C_{18}. A parabolic response was observed with the C_{14} chain length being the most toxic (NOEC = 0.045 mg/l).

There are a number of valid acute toxicity data for many species from all trophic levels available. Taking the data from the whole subcategory into account chronic and subchronic data for all 3 trophic levels are available.

For **alkane sulfonates**, the acute toxicity on *Daphnia magna* has been determined for chain length $C_8 - C_{14}$. Results were comparable to AS in the range between C_8 and C_{10}, while C_{12} and C_{14} are significantly less toxic. Chronic data obtained for C_{12} ASO_3 Na and $C_{12}ASO_4$ Na with the rotifer *Brachionus calicyflorus* similarly show that alkane sulfonates might be less toxic than AS. C_{16} and C_{18} alkane sulfonates are assumed to exhibit the same toxicity than AS of comparable chain lengths. No data are available concerning the toxicity of alkyl sulfonates on fish and algae. However, a similar toxicity might be assumed because of structural and physico-chemical similarities between the three subcategories.

For **α-olefin sulfonates**, reliable short-term tests on fish, invertebrates and algae are available. The results indicate that toxicity is increasing as the alkyl chain length increases. The lowest available effect value is the 96 h-LC_{50} = 0.5 mg/l, determined in tests on *Oryzias latipes*, *Rasbora heteromorpha* and *Salmo trutta*. For several substances of this subcategory the base set was incomplete (only 2 trophic levels covered). The data base for chronic toxicity is also rather small. For the whole subcategory, only one chronic *Daphnia* test, one algae NOEC and 2 subchronic fish tests are available, which were however not conducted with the most toxic substance from the acute tests. In a long-term test with sodium C_{11-14} olefin sulfonate as test substance, NOECs of 1.70 mg/l were determined for early ontogenetic stages of both the loach *Misgurnus fossilis* and the trout *Oncorhynchus mykiss*. In a test on the chronic toxicity to *Daphnia magna*, a NOEC of 4.4 mg/l for C_{14}=/$OHASO_3$ Na was obtained.

The effect of C_{12} ASO_4 Na on natural periphyton communities was assessed in a flow-through laboratory microcosm system. The 28 d-NOEC for algal periphyton communities was 0.055 mg/l. The ecotoxicological response of benthic and lotic microbial and invertebrate stream communities to C_{12} ASO_4 Na was assessed in a P&G experimental stream facility under outdoor conditions. The protozoan species richness increased with test substance concentrations, the 55 d-EC_{20} was determined to be 0.063 mg/l.

Tests on the toxicity to **microorganisms** were only conducted with alkyl sulfates as test substances. A test on the inhibition of respiration of activated sludge resulted in an 3 -h-EC_{50} of 135 mg/l (nominally). The lowest effect value for protozoa was obtained from a test on *Uronema parduczi* using C_{12} ASO_4 Na as test substance, the 20 h-EC_5 was 0.75 mg/l

Experimental test results on benthic organisms in a water-sediment system are not available. However, due to sediment-water partitioning coefficients Kd < 350, no significant risk for organisms in this compartment is to be expected.

For **terrestrial organisms** no valid experimentally derived test results are available. The available toxicity data were

excerpted from insufficiently documented studies. However, the data indicate that toxic effects on soil organisms might only be expected at high concentrations for alkyl sulfates. Toxicity of alkane sulfonates and α-olefin sulfonates can not be assessed because test results for terrestrial organisms are not available.

Exposure

In 2003, alkyl sulfate quantities of totally 118 000 t/a were consumed in the USA and Canada, 105 000 t/a in Western Europe, and 11 500 t/a in Japan.

The consumption of alkane sulfonates in Western Europe (the only significant user of alkane sulfonates) is estimated at 60 000 t/a in 2003.

The consumption of α-olefin sulfonates in Western Europe was about 6000 t/a and in Japan 3000 t/a, while the consumption in the USA and Canada is not reported (2003).

The chemicals of this category are anionic surfactants that are used at typical concentrations between 3 and 5% and up to 20% in consumer cleaning and personal care products, usually in conjunction with other surfactants. They function as laundry and liquid dishwashing detergents, dispersing agents, hard surface cleaners, shampoos, hair conditioners, liquid soaps, cleansing and other personal care products. There are no commercial or industrial process intermediate uses of the chemicals of this category. The predominant disposal route following use of the products that contain chemicals of this category is via wastewater.

Analytical measurements of alkyl sulfates reveal that the concentrations in effluents of waste water treatment plants are mostly below 10 µg/l. In the receiving surface waters, in the 1980s and 1990s, most of the available values were below 5 µg/l, with a maximum of 10.2 µg/l. No monitoring data are available for alkane sulfonates. Concentrations of α-olefin sulfonates (sum of C_{14} to C_{18}) measured in 2004 show a maximum of 0.16 µg/l.

RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health:

This category of chemicals is currently of **low priority** for further work.

These chemicals possess properties indicating a hazard for human health (corrosion/irritation, serious effects on the eye, acute toxicity). These hazards do not warrant further work as they are related to effects which may only become evident at exposure levels that are higher than formulated in consumer products. It should nevertheless be noted by chemical safety professionals and users of the raw materials. In the Sponsor country, occupational exposure is controlled and adequate risk reduction measures are in place by way of Material Safety Data Sheets. Member countries may desire to check their own risk management measures to find out whether there is a need for additional measures.

Environment:

The following chemicals are currently of low priority for further work due to their low hazard profiles:

AS: $C_8 - C_9$ (acute aquatic EC/LC_{50} values >100 mg/l)

PAS: $C_8 - C_{12}$ (acute aquatic EC/LC_{50} values >100 mg/l; chronic aquatic NOEC >1 mg/l)

The following chemicals have properties indicating a hazard for the environment:

AS: $C_{10} - C_{14}$ & C_{18} (acute aquatic EC/LC_{50} values >1 - ≤100 mg/l; NOEC ≤ 1mg/l)

PAS: C_{14} & C_{18} (acute aquatic EC/LC_{50} values >1 - ≤100 mg/l)

AOS: $C_{12} - C_{16}$ (acute aquatic EC/LC_{50} values >1 - ≤100 mg/l)

However they are of low priority for further work for the environment because of their rapid biodegradation under aerobic conditions and their limited potential for bioaccumulation.

The following chemicals have properties indicating a hazard for the environment (acute and chronic aquatic effects at concentrations below 1 mg/l):

AS: $C_{15} - C_{16}$ (acute aquatic EC/LC_{50} values $\leq$1 mg/l, NOEC $\leq$ 1mg/l)

PAS: $C_{15} - C_{16}$ (acute aquatic EC/LC_{50} values $\leq$1 mg/l, NOEC $\leq$ 1mg/l)

AOS: $C_{14-18} - C_{16-18}$ (acute aquatic EC/LC_{50} values $\leq$1 mg/l)

Therefore, they are candidates for further work. Furthermore, member countries are invited to perform an exposure assessment and if necessary a risk assessment.

Note:

The chemicals are supplied commercially under various CAS numbers which describe varying compositions. As a result of this variability it is not possible to state explicitly CAS numbers in the environmental recommendation, rather chain length ranges are used. The toxicity of these mixtures should take into account the toxicities of the individual homologues and their relative amount in the mixture.