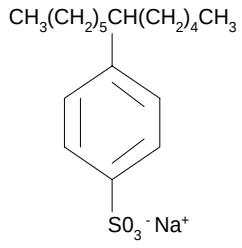
SIDS INITIAL ASSESSMENT PROFILE

CAS Nos.	1322-98-1 Decylbenzene sulfonic acid, sodium salt 25155-30-0 Dodecylbenzene sulfonic acid, sodium salt 26248-24-8 Tridecylbenzene sulfonic acid, sodium salt 27636-75-5 Undecylbenzene sulfonic acid, sodium salt 68081-81-2 C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt 68411-30-3 C_{10-13} Alkylbenzene sulfonic acid, sodium salt 69669-44-9 C_{10-14} Alkyl deriv benzene sulfonic acid, sodium salt 85117-50-6 C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt 90194-45-9 C_{10-13} Alkyl deriv benzene sulfonic acid, sodium salt 127184-52-5 4-C_{10-13}-sec Alkyl deriv. benzene sulfonic acid, sodium salt
Category Name	Linear Alkylbenzene Sulfonate (LAS)
Structural Formula	This structure of a C_{12}-LAS is representative of the category. 

SUMMARY CONCLUSIONS OF THE SIAR

Category Identification/ Justification

The LAS molecule contains an aromatic ring sulfonated at the para position and attached to a linear alkyl chain at any position except the terminal carbons. The alkyl carbon chain typically has 10 to 14 carbon atoms and the linearity of the alkyl chains ranges from 87 to 98%. While commercial LAS consists of more than 20 individual components, the ratio of the various homologs and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain, is relatively constant in currently produced products, with the weighted average carbon number of the alkyl chain based on production volume per region between 11.7-11.8. LAS are supported as a category because of the close consistency of the mixtures, their commercial uses, fate, and health and environmental effects. LAS is the primary cleaning agent used in many laundry detergents and cleaners at concentrations up to 25 percent in consumer products, and up to 30 percent in commercial products, with the exception of one reported product at 45% percent in concentrated solid form that is mechanically dispensed into diluted solution for dishwashing.

Human Health

Substantial data exist for mammalian toxicity. The available data indicate that LAS exhibits slight acute toxicity. Oral LD_{50} values for rats range from 1,080 to 1,980 mg/kg bw. Oral LD_{50} values for mice are 2,160 and 2,250 mg/kg bw for males and females, respectively. The rat dermal LD_{50} value was greater than 2,000 mg/kg bw. The oral and dermal acute toxicity data for LAS generally indicate low hazard potential when all studies are considered together. Acute inhalation toxicity data indicate that LAS is moderately toxic, with mortality occurring at respirable particle concentrations of 310 mg/m^3 (MMAD = 2.5 microns).

In a series of studies on rabbits, LAS was not irritating to the skin or eyes at low concentrations (0.5-2.5%), moderately irritating at 5%, and more severely irritating at higher (about 50%) concentrations. In studies that included rinsing, eye irritation effects diminished with rinsing after 30 seconds of exposure and were slight with rinsing after 4 seconds of exposure. In a low volume eye test (LVET) using a 35% LAS solution, rabbits experienced moderate irritation that was completely reversible by day 35. (Note that the maximum concentration of LAS is 25 percent in consumer products and normally less than 30 percent in commercial products.) Accidental eye exposure in 231 manufacturing employee incidents and 284 consumer incidents established that eye irritation effects of exposure during manufacturing and use of products containing LAS and other surfactants are moderate, transient and reversible.

In 15 repeated dose studies with rats, mice, and monkeys exposed to LAS via oral and dermal routes, LOAELs ranged from 115 to 750 mg/kg bw/day. The corresponding NOAELs ranged from 40 to 250 mg/kg bw/day. Effects commonly observed included suppressed body weight gain, diarrhea, increases in relative liver weight, differences in enzymatic and serum-biochemical parameters, and mild degeneration and desquamation of the tubular epithelium in the kidneys.

In four well designed *in vitro* bacterial (*Salmonella*) mutagenicity studies, LAS shows no evidence of mutagenicity either with or without S9 metabolic activation. LAS showed no evidence of causing increased cell transformation in an *in vitro* cell transformation assay. In *in vivo* studies, no significant differences in chromosome aberrations were seen when mice were given either oral doses up to 800 mg/kg bw/day or dietary doses up to 1170 mg/kg bw/day. In a mouse micronucleus study, LAS did not induce a clastogenic effect. Rats given dietary doses up to 450 mg/kg bw/day also showed no significant differences in chromosome aberrations. Collectively, these data support that LAS is not genotoxic.

The highest dose tested in four carcinogenicity studies with rats was 300 mg/kg bw/day. In the most documented study, rats were administered up to 250 mg LAS/kg body weight/day in the diet for two years. Results of this study indicate no gross or histopathological evidence of a carcinogenic effect. No evidence of tumorigenesis was observed in any of the carcinogenicity studies. While the quality and focus of the studies precludes a definitive assessment, the results of the genetic toxicology and rodent bioassay studies collectively provide strong weight-of-evidence support that LAS is not genotoxic and is not a rodent carcinogen.

Similarly, no evidence of reproductive or fertility effects was observed in any of the three available reproductive toxicity studies in which rats were given dietary doses over three to four generations. NOAELs from these reproductive studies ranged from 70 to 350 mg/kg bw/day, which were the highest doses tested. In 17 developmental toxicity studies, effects such as embryo death or deformities, and litter loss were most often observed only at maternally toxic doses and were associated with the irritation effects of LAS on skin or the gastrointestinal tract. No decreases in litter size, no changes in litter parameters, no malformations or significant differences in skeletal defects were observed at oral doses up to 780 mg/kg bw/day in rats and at dermal doses of 500 mg/kg bw/day in mice and 90 mg/kg bw/day in rabbits.

All of the studies included in the dossier are considered reliable, but all with limitations. The results are consistent with each other and these data are used in a weight-of-evidence approach. Based on these considerations, the highest NOAEL value below the lowest LOAEL from all of the mammalian toxicity studies is the most appropriate. Therefore, the NOAEL is 85 mg/kg bw/day. This value comes from a rat drinking water, 9-month repeated dose toxicity study. The lowest LOAEL (115 mg/kg/day) was associated with increased weight of the cecum and slight degeneration of the renal tubules.

Environment

Pure LAS is a solid at ambient temperatures with a melting point of 198.5°C. The boiling point for LAS could not be determined experimentally due to decomposition beginning at 444°C. LAS has a low vapor pressure (calculated as 3-5 x 10^{-13} Pa). LAS is water soluble, with a critical micelle concentration (CMC) value of 0.1 g/L and forms a clear solution in water at concentrations up to 250 g/L. Although it is impossible to accurately measure an octanol-

water partition coefficient for surface-active agents like LAS, an octanol-water partition coefficient of log 3.32 has been calculated for $C_{11.6}$ LAS. K_d values for LAS in activated sludge and sediment increased with increasing alkyl chain length of LAS homologues with K_d values for C_{12} LAS of 3210 L/kg in activated sludge and 330 L/kg in river sediment. In activated sludge, sorption and desorption equilibria for LAS were achieved very rapidly, and comparison of the extent of sorption and biodegradation shows that the absorbed fraction as well as the soluble fraction of LAS is available for biodegradation. Based on Fugacity III modeling results using the most relevant input parameters, more than 99 percent of the residual (non-biodegraded) fraction of LAS distributes to the soil. LAS does not undergo significant degradation by abiotic mechanisms under environmentally relevant conditions as photolyzable and hydrolyzable groups are absent from the chemical structure.

An extensive database of studies demonstrates rapid and complete (ultimate) biodegradation of LAS in many of the available aerobic biodegradation tests, including soil and the aqueous environment. In several tests, LAS has been shown to be readily biodegradable, and has passed the 10-day biodegradation window in mineralization tests for most ready tests. LAS is removed in biological wastewater treatment at percentages ranging from 77-82% for trickling filters up to 99%+ for activated sludge. The biodegradation kinetics of the longer alkyl chain lengths are generally faster, and their sorption coefficients larger. The primary degradation intermediates are sulfophenyl carboxylates (SPCs), which further degrade to CO_2, SO_4^{2-}, and water. LAS does not generally degrade under anaerobic conditions. The measured bioconcentration factors of pure homologues and isomers decrease with decreasing average alkyl chain lengths (from almost 1000 for 2-phenyl-C_{13} LAS to 2 for 6-phenyl-C_{10} LAS), all with rapid clearance. The calculated BCF for currently produced $C_{11.6}$ LAS is 87 and was 22 for filtered Mississippi River water (average alkyl chain length of surface water fingerprint = $C_{10.8}$).

Ecotoxicity data are extensively available for LAS, with several comprehensive reviews having been completed. The lowest reliable acute $LC_{50}/EC_{50}/ErC_{50}$ values based on a review of the aquatic toxicity data on commercially representative LAS ($C_{11.6}$-$C_{11.8}$) were 1.67, 1.62 and 29.0 mg/L for fish, *Daphnia magna*, and algae, respectively. Acute toxicity is greater for individual LAS homologues with longer alkyl chain lengths. LAS biodegradation intermediates are significantly less toxic than the parent LAS with L/EC_{50} values >1000 mg/L for fish and *D. magna*. Chronic freshwater toxicity studies following guideline exposures (28-30 days for fish, 21 days for invertebrates and 3-4 days for algae provided the following NOEC values: fish NOEC = 1 mg/L (two studies, two species); Daphnia, NOEC = 1.18-3.25 mg/L (six values, two studies, one with 5 diets); algae, NOEC = 0.4-18 mg/L (four studies, two species). In addition all of the available, reliable chronic single species aquatic toxicity data on LAS have been evaluated, including three freshwater species in which multiple studies were reported and nine freshwater species for which single studies were reported. Single NOEC values and geometric mean NOEC values (calculated for species with multiple results) were normalized to $C_{11.6}$ LAS. These NOEC values range from 0.25 to 6.1 mg/L for freshwater species, including fish, invertebrates, algae and higher plants. Geometric mean NOEC values for marine species ranged from 0.025 to 5.0 mg/L. Based on the model ecosystem studies, a NOEC of 0.27 mg/L (0.37 if normalized to $C_{11.6}$ LAS) was determined for the freshwater ecosystem. This value is based on model stream ecosystem studies of over 250 species, and is consistent with the single species chronic freshwater data.

NOEC values for sediment exposures were greater than or equal to 81 mg/kg dry matter based on studies in four species, including GLP studies in *L. variegates* (survival, reproduction and growth over 28 days) and *C. elegans* (egg production, 3 days). Field studies indicate no adverse effects of LAS in sludge-amended soil from LAS levels of 15 mg/kg dry matter in the soil (9 microbial functions/processes and abundance/diversity of microarthropods and earthworms, short-term and 4 years) or 31,300 mg/kg dry matter in sludge (function of microbial community, short-term and 1 year).

In laboratory studies in which young trees are exposed to artificial sea spray, LAS concentrations of 10 mg/L lead to increased foliar penetration of NaCl, a hypothesized mechanism of defoliation.

A health and environmental risk assessment is available (heraproject.com).

Exposure

Current LAS production is approximately 390,000 metric tons in the North America, 400,000 metric tonnes in

Europe, and 85,000 metric tonnes in Japan. Global production was 2.6 million metric tonnes in 1995. In the production phase, manufacturing processes have been designed to maximize production yield and minimize potential releases. Worker exposure is possible during the detergent formulation stage by inhalation of powders or dermal contact of powders and liquids. Good manufacturing design practices (e.g., enclosed production in agglomeration processes, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) in place at facilities that manufacture liquid and dry (granular/powder) materials are anticipated to mitigate worker exposure to LAS. Any LAS that is not incorporated into a product is captured by dust-handling equipment for recycling back into the production process. A limited amount of LAS in aqueous solution may be released as a dilute solution from washing and rinsing operations in the manufacturing process and is discharged to wastewater treatment. Incidental quantities of the dry (granular/powder) product (e.g., from floor sweepings) may be disposed in landfills.

Labeling of consumer products containing LAS and other surfactants include warnings of the potential for eye irritation and first aid instructions to rinse with water.

Data suggest that inhalation of LAS products during use will be low. Spray products containing LAS are designed to produce the large particle sizes needed for efficient delivery of the spray to the surface being cleaned. In laboratory simulations with six spray nozzles representing those used in spray cleaning products, less than 0.1% of the total volume sprayed consists of respirable particles (particles under 10 microns in diameter) and air concentrations in the breathing zone are in the 0.13-0.72 mg/m^3 range. Inhalation of detergent dusts during washing processes, modeled by HERA (2004), was 10-fold lower than inhalation of aerosols from cleaning product sprays. This estimate is based on a published study reporting an average of 0.27 µg dust per cup of product used for machine laundering. This is a conservative (protective) estimate as exposure from modern compact/granular detergent formulations produced in agglomeration processes, which produce larger particle sizes, would be expected to be much less. Based on these data, it is expected that exposures to respirable particles from inhalation are low.

Results of extensive environmental monitoring evaluations in the United States indicate that measured surface water concentrations were generally below 50 µg/L for river water samples collected under low dilution (worst case) conditions below treatment plant mixing zones. Values in the 2800 km reach of the Mississippi River from Minneapolis to New Orleans range from non-detect (<0.1 µg/L) to 28 µg/L (362 samples). LAS river water concentrations similar to those in the US were observed in monitoring studies conducted in Europe and Japan.

Measured LAS concentrations in river sediments were generally less than 1-2 mg/kg dry weight. Mississippi River sediments were <1 mg/kg dry matter with one exception. LAS levels in sediments of the receiving waters of the Tiber River (Italy) were 1.8 mg/kg dry matter. Higher LAS concentrations have been observed near untreated or poorly treated wastewater discharges, e.g. LAS in sediments of a small river (Rapid Creek, USA) below a trickling filter treatment plant averaged 190 mg/kg just below the outfall, 11.2 mg/kg less than 5 miles downstream and 5.3 mg/kg greater than 5 miles downstream

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

Human Health: The chemicals in the LAS category are currently of low priority for further work because of their low hazard potential except for skin and eye irritation and acute inhalation. Based on data presented by the Sponsor Country, exposure to respirable particles is anticipated to be low. Other countries may desire to investigate any exposure scenarios that were not presented by the Sponsor Country.

Environment: The chemicals in the LAS category possess properties indicating a hazard for the environment (fish, invertebrates and algae). However, they are of low priority for further work due to ready and/or rapid biodegradation and limited potential for bioaccumulation.