Secondary alkane sulfonates (SAS): Human health tier II assessment

27 November 2014

Chemicals in this assessment

Chemical Name in the Inventory	CAS Number
Sulfonic acids, C10-18-alkane, sodium salts	68037-49-0
Sulfonic acids, C13-18-sec-alkane, sodium salts	75534-59-7
Sulfonic acids, C13-17-alkane, sodium salts	93763-92-9
Sulfonic acids, C12-18-sec-alkane, sodium salts	106233-08-3

Preface

This assessment was carried out by staff of the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) using the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework.

The IMAP framework addresses the human health and environmental impacts of previously unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory).

The framework was developed with significant input from stakeholders and provides a more rapid, flexible and transparent approach for the assessment of chemicals listed on the Inventory.

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS

already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

The IMAP framework is a science and risk-based model designed to align the assessment effort with the human health and environmental impacts of chemicals. It has three tiers of assessment, with the assessment effort increasing with each tier. The Tier I assessment is a high throughput approach using tabulated electronic data. The Tier II assessment is an evaluation of risk on a substance-by-substance or chemical category-by-category basis. Tier III assessments are conducted to address specific concerns that could not be resolved during the Tier II assessment.

These assessments are carried out by staff employed by the Australian Government Department of Health and the Australian Government Department of the Environment and Energy. The human health and environment risk assessments are conducted and published separately, using information available at the time, and may be undertaken at different tiers.

This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

For more detail on this program please visit:**www.nicnas.gov.au**

Disclaimer

ACRONYMS & ABBREVIATIONS

Grouping Rationale

This group of chemicals contains anionic surfactants that are manufactured by sulfoxidation of n-paraffins (HERA, 2005). They have very good water solubility, a high wetting action, a pronounced foaming power and excellent grease and soil dispersing properties, making them important surfactant ingredients in detergents, especially for dish washing.

Even though the physical–chemical behaviour of these chemicals might be influenced by different counterions, they are not expected to affect the chemical reactivity and the hazard classification for the purpose of this assessment.

Given the close structural similarities and surfactant properties of these chemicals, very similar hazard profiles for human health are expected. They also have similar reported uses.

Import, Manufacture and Use

Australian

No specific Australian use, import, or manufacturing information has been identified.

International

The following international uses have been identified through Galleria Chemica; Substances and Preparations in Nordic countries (SPIN) database; Household Products Database and Human and Environmental Risk Assessment (HERA) on ingredients of household cleaning Products (HERA, 2005):

The chemicals in this group have the following reported cosmetic uses in:

- hair shampoos;
- shower gels;
- foam baths (concentration 0.002 %);
- liquid soaps (concentration 1–3 %); and
- emulsions and toothpastes.

The chemicals in this group have the following reported domestic uses as surface-active agents including in:

- household detergents;
- laundry detergents;
- hand wash (concentration <1 %);
- dishwashing products (concentration <2.5 %); and
- household cleaning products.

The chemical has the following reported commercial uses as surface-active agents including:

- as a wool-washing agent;
- as an active ingredient in both light- and heavy-duty laundry formulations (upholstery formulations);
- as an emulsifier for lubricants and penetrants in varnish and paint remover;
- in adhesives and binding agents; and
- in site limited uses as a corrosion inhibitor in metal processing.

The following non-industrial uses have also been identified:

- as an emulsifier, whipping agent and surfactant in foods;
- as an emulsifier, wetting agent and adjuvant in insecticides; and
- in non-agricultural pesticides and preservatives.

Restrictions

Australian

No known restrictions have been identified.

International

No known restrictions have been identified.

Existing Worker Health and Safety Controls

Hazard Classification

The chemicals are not listed on the Hazardous Substances Information System (HSIS) (Safe Work Australia).

Exposure Standards

Australian

No specific exposure standards are available.

International

No specific exposure standards are available.

Health Hazard Information

The chemicals in this group have overlapping carbon chain lengths. Another chemical with overlapping chain length range, C14-17-sec-alkane, sodium salts (CAS No. 97489-15-1) is not on the Australian Inventory of Chemical Substances (AICS). However, in the absence of study data on the chemicals in the group, data from this non-AICS chemical are used as it is an appropriate analogue (HERA, 2005).

Toxicokinetics

Chemicals in this group are absorbed through skin during use in cosmetics and toiletries and via oral ingestion, e.g. by using a surfactant-containing toothpaste; through residues from dishwashing detergents; and through traces of surfactants in potable water (Dekker, 1992).

Anionic surfactants are generally well absorbed in the intestine and are distributed mainly to the liver. The metabolic degradation of the linear alkyl chain is instigated by beta-oxidation. After absorption, a part of the chemical is excreted via bile, in the faeces. The majority of metabolites are rapidly excreted in urine (Sterzel & Dusseldorf, 2005).

Acute Toxicity

Oral

The group of chemicals has moderate acute oral toxicity. In animal tests, the analogue chemical had median lethal doses (LD50) in the range of 500–2000 mg/kg bw. These data warrant hazard classification for the members of this group.

The acute oral toxicity of SAS 60 (CAS No. 97489-15-1)(60 % active content) was investigated in rats. Ten female SPF-Wistar rats were administered the chemical by oral gavage at doses of 1600, 2500 or 4000 mg/kg bw. Following application, the animals were observed for seven days. At the highest dose all animals died and at the mid-dose 3/10 animals died. Necropsy showed reddened intestinal tract mucosa and enlargement of the caecum. The LD50 was calculated to be 2890 mg/kg bw (REACH).

In another study, 500 or 2000 mg/kg bw SAS 93 (CAS No. 97489-15-1) (93 % active content) was administered to five males and five female Wistar rats per dose. The animals were observed for 14 days following treatment. No deaths occurred at 500 mg/kg bw. However, all animals died at 2000 mg/kg bw. Reported signs of toxicity included stomach full of a reddish-black mass, intestinal tract filled with reddish mucous and lungs partly filled with blood. The LD50 was determined to be 500–2000 mg/kg bw.

Dermal

No data are available for the chemicals.

Inhalation

No data are available for the chemicals.

Corrosion / Irritation

Skin Irritation

Based on the available information on the analogue chemical, the chemicals in this group (CAS No 97489-15-1 and CAS No. 68037-49-0) should be considered to be skin irritants.

In an irritation study conducted according to the Organisation for Economic and Co-operative Development Test Guideline (OECD TG) 404 in three female New Zealand White rabbits, 0.5 mL of undiluted SAS 60 (CAS No. 97489-15-1; 60 % active content) was applied dermally for four hours. Severe erythema and very slight to moderate oedema were observed up to seven days after removal of the patches. The skin of all animals was indurated, discoloured brown and chapped. After the observation period of 14 days, all signs of irritation had completely resolved (REACH).

In an another irritation study conducted according to OECD TG 404 on three New Zealand White rabbits, 0.5 g of undiluted SAS 93 (CAS No. 97489-15-1; 93 % active content) was applied dermally for four hours. Oedema and erythema were observed in all animals up to seven days after removal of the patches. All the signs were completely reversed after seven days (REACH).

Eye Irritation

Based on the available information on the analogue chemical, the chemicals in this group are likely to cause severe eye damage.

In an eye irritation study conducted according to OECD TG 405, 0.1 mL of undiluted SAS 30 (CAS No. 97489-15-1; 30 % active content) was applied into the left conjunctival sac of one New Zealand White rabbit then observed for seven days. It was reported moderate eye irritation, including corneal and iridial effects, and that these effects were not reversed after seven days (REACH).

In another study conducted according to OECD TG 405, 0.1 mL of undiluted SAS 60 (CAS No. 97489-15-1; 60 % active content) was tested in three White Russian rabbits. Severe irritation, including corneal and iridial effects, was not reversed after 21 days (REACH).

Observation in humans

The chemical SAS 60 (CAS No. 97489-15-1; 60 % active content) was tested for skin irritation in 15 test human volunteers with healthy skin. The volunteers were dermally exposed in an open patch test for 15 minutes. Very slight itching was reported in two test volunteers, whereas the remaining 13 volunteers had no adverse effects.

Sensitisation

Skin Sensitisation

Based on the available information, the chemicals in this group are not skin sensitisers.

A guinea pig maximisation study was conducted according to OECD TG 406. In the screening study, the highest non-irritating concentration of SAS 60 (CAS No. 97489-15-1; 60 % active content) was 5 % in water. In the main study 15 male Pirbright White guinea pigs were used. Exposure included intradermal induction at 0.05 mL of a solution of 500 mg of the chemical in 10 mL of Freund's complete adjuvant. The animals were challenged 14 days later with 5 % SAS 60(CAS No. 97489-15-1; 60 % active content). There were no signs of skin reactions (REACH).

Repeated Dose Toxicity

Oral

Based on the available data, the chemicals in this group are not considered to cause serious damage to health on repeated oral exposure. A no observed adverse effect level (NOAEL) of 0.4 % SAS 60 (CAS No. 97489-15-1; 60 % active content), equivalent to 200 mg/kg bw/day, was established in a one year study.

SAS 60 (CAS No. 97489-15-1; 60 % active content) was investigated in a one-year feeding study for repeated dose toxicity. Sprague Dawley (SD) rats (30 animals/sex/dose) were treated with 0, 40, 200 or 1000 mg/kg bw/day SAS 60. Ten male and female rats from each group were euthanised for an interim examination after 26 weeks. No signs of toxicity were seen at treatment levels of 200 mg/kg bw/day and below. Body weights were reduced in rats treated at 1000 mg/kg bw/day of the chemical. Macro- and microscopic examinations of rats killed after 26 or 52 weeks revealed no changes in morphology attributable to the treatment (REACH). Therefore, the NOEL was 0.4 % (equivalent to 200 mg/kg bw/day).

Dermal

Based on the available data, the chemicals in this group are not considered to cause serious damage to health on repeated dermal exposure.

In a dermal toxicity study, SAS 60 (CAS No. 97489-15-1; 60 % active content) was topically administered at initial doses of 0, 50, 250 or 500 mg/kg bw/day to CD-1 mice (25 females/group). In the highest dose groups, doses were increased as high as 8000 and 16000 mg/kg bw during the course of the study. Treatment was for five days per week for four or five consecutive weeks for various groups. Dermal irritation was observed in all mice within two days of treatment starting at dose 16,000 mg/kg bw/day (32 % SAS 60 (w/v)). At 8000 mg/kg bw/day (16 %, SAS 60 (w/v)) mice showed skin thickening after one week of treatment. Mice treated with 4000 mg/kg bw/day SAS 60 and below did not show skin irritation. Absolute and relative spleen weights were increased in mice treated with the highest dose. However, this is considered a secondary response to inflammation. The reported no observed adverse effect level (NOAEL) for local effects was 500 mg/kg bw/day, and for systemic effects 1000 mg/kg bw/day (REACH).

Inhalation

No data are available.

Genotoxicity

The chemicals of this group are not genotoxic based on results from in vitro or in vivo studies.

In vitro studies

Available data for SAS (CAS No: 97489-15-1 and CAS No.68067-49-0) indicate that the chemicals are not mutagenic in bacterial assays (OECD TG 471) with and without metabolic activation or in a mammalian cell HPRT locus test.

In an Ames test, 0.001–5 µL/plate SAS 30 (CAS No. 97489-15-1; 30 % active content) was investigated for point mutations in the strains TA 98, TA 100, TA 1535 and TA 1537 with and without metabolic activation in *Salmonella typhimurium* (REACH).

In a mammalian cell gene mutation assay according to OECD TG 476, SAS 93 (CAS No. 97489-15-1; 93 % active content) was non-mutagenic in the hypoxanthine-guanine-phosphoribosyl-transferase (HPRT) locus assay using Chinese Hamster V79 cells (REACH).

In vivo studies

In a chromosomal aberration assay, SAS 60 (60 % active content) was fed to NMRI (Naval Medical Research Institute) male and female mice (five animals/group) at 600, 1200 or 2400 mg/kg bw over 24 hours. Chromosome preparations were made from the bone marrow (femur) of eight animals per day over several days. The chemical had no effect on structural chromosomal aberration in the treatment groups (REACH).

Carcinogenicity

Based on the available data from rat and mouse studies on the analogue chemical, there is no indication for the potential carcinogenicity of chemicals in this group.

In a carcinogenicity study, CD rats (50 animals/sex/dose) were fed diets containing 0, 40, 200 or 1000 mg/kg bw/day of SAS 60 (CAS No. 97489-15-1; 60 % active content) for two years. No tumour related findings were noted (REACH).

In another carcinogenicity study, 0, 0.1, 0.5 or 1 % (w/v) SAS 60 (CAS No. 97489-15-1; 60 % active content) was topically administered to the shaved backs of CD-1 mice (100 animals/sex/dose) for 80 weeks. No tumour related findings were reported in this study (REACH).

Reproductive and Developmental Toxicity

Reproductive and developmental toxicity effects were not observed for the analogue.

A two-generation study was carried out in male and female Charles River CD rats. Male and female rats were exposed to SAS 60 (CAS No. 97489-15-1; 60% active ingredient) (100, 300 or 1000 mg/kg bw/day) by oral gavage daily for 60 days before mating, during mating and through weaning of the first generation (F1) offspring. The F1 parental animals were exposed from postpartum day 22 until the end of the study. Parents in the F1 generation did not show any signs of reproductive toxicity, but were reported to have a slight, not statistically significant, reduction in body weight (male rats at 1000 mg/kg bw/day). There were no treatment-related signs of reproductive toxicity noted in the second generation (F2). The NOAEL for reproductive and developmental toxicity is reported as 500 mg/kg bw/day (REACH).

Risk Characterisation

Critical Health Effects

The critical health effects for risk characterisation are systemic acute effects (acute toxicity after oral exposure) and local effects (skin and eye irritation).

Public Risk Characterisation

The chemicals in this group have reported cosmetic and domestic uses in Australia and overseas. Australian and overseas information suggests that the chemicals are generally used at low concentrations in cosmetics and up to 15 % for domestic purposes. The HERA (2005) states that the highest volume use for the chemicals in Europe is in dishwashing liquid (concentration <2.5 %).

Based on the critical health effects identified for these chemicals, the highest concern relates to eye irritation. While there is potential for ocular exposure in a domestic setting, this is not likely to be a concern at the low concentrations in identified domestic products in Australia and overseas. Based on the available eye irritation studies, the analogue chemical (CAS No. 97489-15-1) at 15 % may be irritating in a similar manner to other anionic surfactants. The chemicals are not considered to pose a greater risk to public health compared with the other commonly available anionic surfactants.

Occupational Risk Characterisation

During product formulation, oral, dermal and ocular exposure of workers to the chemicals in this group might occur, particularly where manual or open processes are used. These can include transfer and blending activities, quality control analysis, and cleaning and maintenance of equipment. Worker exposure to the chemicals at lower concentrations could also occur while using formulated products containing the chemical. The level and route of exposure will vary depending on the method of application and work practices employed.

Given the critical systemic acute and local health effects, the chemicals in this group may pose an unreasonable risk to workers unless adequate control measures to minimise oral, dermal and ocular exposure to the chemicals are implemented. The chemicals should be appropriately classified and labelled to ensure that a person conducting a business or undertaking (PCBU) at a workplace (such as an employer), has adequate information to determine appropriate controls.

The data available support an amendment to the hazard classification in the Hazardous Substances Information System (HSIS) (Safe Work Australia) (refer to **Recommendation** section).

NICNAS Recommendation

Assessment of these chemical are considered to be sufficient, provided that the recommended amendment to the classification is adopted, and labelling and all other requirements are met under workplace health and safety and poisons legislation as adopted by the relevant state or territory. While evidence from studies on the analogue chemical suggest that additional public health controls may be warranted to protect against eye irritation from the chemicals in this group, such effects are likely to relate to the total concentration of anionic surfactants in a product rather than the concentration of an individual chemical alone.

Regulatory Control

Work Health and Safety

The chemical is recommended for classification and labelling under the current approved criteria and adopted GHS as below. This assessment does not consider classification of physical and environmental hazards.

Hazard	Approved Criteria (HSIS)[a]	GHS Classification (HCIS)[b]
Acute Toxicity	Harmful if swallowed (Xn; R22)	Harmful if swallowed - Cat. 4 (H302)
Irritation / Corrosivity	Risk of serious eye damage (Xi; R41) Irritating to skin (Xi; R38)	Causes serious eye damage - Cat. 1 (H318) Causes skin irritation - Cat. 2 (H315)

[a] Approved Criteria for Classifying Hazardous Substances [NOHSC:1008(2004)].

[b] Globally Harmonized System of Classification and Labelling of Chemicals (GHS) United Nations, 2009. Third Edition.

[*] Existing Hazard Classification. No change recommended to this classification

Advice for industry

Control measures

Control measures to minimise the risk from oral, dermal and ocular exposure to the chemicals should be implemented in accordance with the hierarchy of controls. Approaches to minimise risk include substitution, isolation and engineering controls. Measures required to eliminate, or minimise risk arising from storing, handling and using a hazardous chemical depend on the physical form and the manner in which the chemicals are used. Examples of control measures which could minimise the risk include, but are not limited to:

- using closed systems or isolating operations;
- minimising manual processes and work tasks through automating processes;
- work procedures that minimise splashes and spills;
- regularly cleaning equipment and work areas; and
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemicals.

Guidance on managing risks from hazardous chemicals are provided in the *Managing risks of hazardous chemicals in the workplace—Code of practice* available on the Safe Work Australia website.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

Obligations under workplace health and safety legislation

Information in this report should be taken into account to help meet obligations under workplace health and safety legislation as adopted by the relevant state or territory. This includes, but is not limited to:

- ensuring that hazardous chemicals are correctly classified and labelled;
- ensuring that (material) safety data sheets ((M)SDS) containing accurate information about the hazards (relating to both health hazards and physicochemical (physical) hazards) of the chemicals are prepared; and
- managing risks arising from storing, handling and using a hazardous chemical.

Your work health and safety regulator should be contacted for information on the work health and safety laws in your jurisdiction.

Information on how to prepare an (M)SDS and how to label containers of hazardous chemicals are provided in relevant codes of practice such as the *Preparation of safety data sheets for hazardous chemicals—Code of practice* and *Labelling of workplace hazardous chemicals—Code of practice*, respectively. These codes of practice are available from the Safe Work Australia website.

A review of the physical hazards of these chemicals has not been undertaken as part of this assessment.

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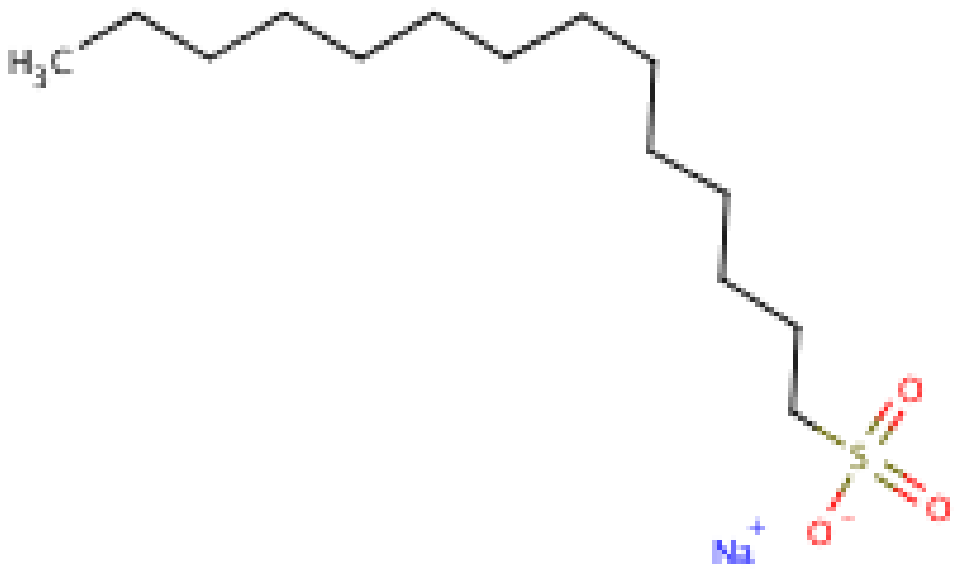
Chemical Identities

Chemical Name in the Inventory and Synonyms	**Sulfonic acids, C10-18-alkane, sodium salts** (C10-18) n-Alkyl sulfonic acids, sodium salts Secondary n-alkane, sulfonate Volgonat
CAS Number	68037-49-0
Structural Formula	

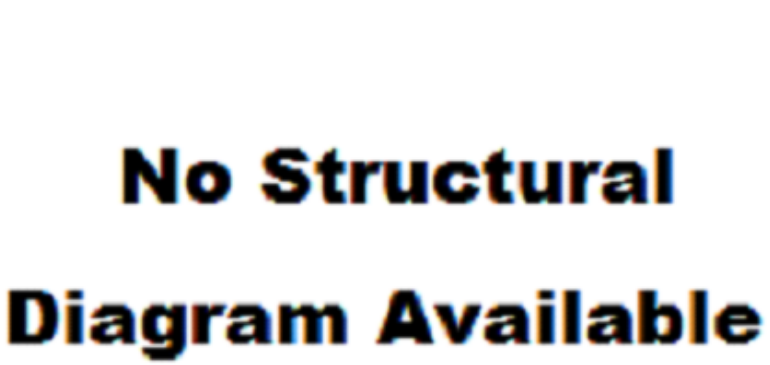
	
Molecular Formula	Unspecified
Molecular Weight	300.44

Chemical Name in the Inventory and Synonyms	**Sulfonic acids, C13-18-sec-alkane, sodium salts** Sulfonic acids, c13-18-sec-alkane, sodium salts
CAS Number	75534-59-7
Structural Formula	**No Structural Diagram Available**

Molecular Formula	Unspecified
Molecular Weight	N/A

Chemical Name in the Inventory and Synonyms	**Sulfonic acids, C13-17-alkane, sodium salts**
CAS Number	93763-92-9
Structural Formula	**No Structural Diagram Available**
Molecular Formula	Unspecified
Molecular Weight	N/A

Chemical Name in the Inventory and Synonyms	**Sulfonic acids, C12-18-sec-alkane, sodium salts**
CAS Number	106233-08-3
Structural Formula	

	
Molecular Formula	Unspecified
Molecular Weight	N/A

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