201-14187A

High Production Volume (HPV) Chemical Challenge Program
Hazard Data Availability and Assessment Report
for
Linear and Branched Alkylbenzene Sulfonic Acids and Derivatives

Prepared on behalf of
The LAS/ABS Consortium

December 27, 2002

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1.0 Introduction

This hazard data availability and assessment is for a group of linear and branched alkylbenzene sulfonates (LAS/ABS) classified as high production volume (HPV) chemicals according to criteria established by the United States Environmental Protection Agency's (U.S. EPA) HPV Chemical Challenge Program, i.e., >1,000,000 pounds manufactured in or imported into the U.S. annually. Six chemicals, each described by a Chemical Abstract Service Registration Number (CAS RN), are indicated in Table 1-1 as chemicals A to F and are produced/imported into the U.S. at about 35,000,000 pounds (U.S. EPA 1990 Inventory Update Rule) on an annual basis. LAS/ABS chemicals are anionic surfactants used to lower the surface tension of water. These chemicals are used in cleaning products for home, institutional and industrial use, e.g. car wash liquids, laundry detergents, liquid dish detergents, hard surface cleaners, dry cleaning products, waterless hand cleaners, and industrial cleaners. They are also used in emulsion polymerisation (e.g., some agriculture products), as dye dispersants in the textile industry, in paint strippers, in some specialized personal care products**,** and for 'bubble making' solutions in children's products. Commercial products usually contain 60-90% LAS/ABS and consumer products 5-30% LAS/ABS.

Table 1-1 Sponsored Chemicals

CAS RN		**Chemical Name**
26264-05-1	A	Benzenesulfonic acid, dodecyl-, compd. with 2-propanamine (1:1)
27323-41-7	B	Benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris[ethanol](1:1)
26264-06-2	C	Benzenesulfonic acid, dodecyl-, calcium salt
68411-32-5	D	Benzenesulfonic acid, dodecyl-, branched
68608-88-8	E	Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.
68953-96-8	F	Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts

These six chemicals (identified as HPV chemicals in 1990 IUR reporting) are being sponsored by the Soap and Detergent Association (SDA)-managed LAS/ABS Consortium. Because of nomenclature modifications adopted to provide more descriptive characterization of the chemical entities, two of the sponsored chemicals are now identified by additional chemical names and CAS registration numbers. Specifically. It should be noted that:

- The commercial substance benzenesulphonic acid, dodecyl-, compd. with 2-propanamine (sponsored Substance "A", CAS RN 26264-05-1) is also known as benzenesulfonic acid, C10-16-alkyl derives., compds. with 2-propanamine, linear (CAS RN 68584-24-7), and as benzenesulfonic acid, dodecyl-, branched , compds. with 2-propanamine, branched (CAS RN 90218-35-2).
- The commercial substance benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris[ethanol](1:1) (sponsored Substance "B" CAS RN 27323-41-7) is also known as benzenesulfonic acid, C10-13-alkyl derives., compds. with triethanolamine, linear (CAS RN 68411-31-4), and as benzenesulfonic acid, dodecyl, branched, compds. with triethanolamine, branched (CAS RN 70528-84-6).

Both the "old" chemical names and CAS RN and the "new" chemical names and CAS RN are currently in use and describe the same chemical entities in commerce before and after the 1990 IUR listing.

The Consortium is committed to assemble and review available public and private Organization for Economic Cooperation and Development (OECD) Screening Information Data Set (SIDS) endpoint data and to develop an assessment plan for the sponsored chemicals. The Consortium is comprised of SDA member companies and includes:

Akzo Nobel Surface Chemistry LLC
Baker Petrolite Corporation
Goldschmidt Chemical Corporation
Harcros Chemicals Inc.
Rhodia Inc.
Stepan Company

This assessment focuses on available publicly and privately held data for the six sponsored chemical entities that share close structural and behavioral similarities. SIDS endpoint data for two additional 'supporting chemicals' are also currently included in this assessment. However, the data availability analysis (and corresponding data gap analysis and final assessment plan) should not be considered complete at this time as additional information that can be utilized to support the category is currently under preparation by other HPV consortia. These additional data sources include: (1) the Linear Alkylbenzene Sulfonate (LAS) Category sponsored by the Industry Coalition for the SIDS Assessment of LAS (in accordance with the International Council of Chemical Associations (ICCA) High Production Volume Chemical Initiative), and (2) the Linear Alkylbenzene (LAB) Sulfonic Acid Category sponsored by the LAB Sulfonic Acid Coalition (in accordance with the U.S. HPV Challenge Program). Once the assessments for the LAS and LAB Sulfonic Acid categories are complete, some of their data will be used to further support the six chemicals in this assessment. This will be accomplished by revising this assessment to incorporate additional read-across data and descriptions, where appropriate.

The use of read-across data from the two "supporting chemicals" that are currently included, as well as from known-to-be structurally and behaviorally similar chemicals in the LAS and LAB Sulfonic Acid categories, are expected to provide for a much more efficient evaluation of the proposed LAS/ABS category.[1] The LAS/ABS Consortium believes that this additional data, when made available, will significantly reduce the number of suggested animal tests (where data are not available and a knowledge gap is indicated).[2] The LAS/ABS Consortium is committed to completing this

[1] The supporting chemicals include: benzenesulfonic acid, linear alkyl (42615-29-2), benzenesulfonic acid, linear alkyl, magnesium salt (68584-26-9), benzenesulfonic acid, C10-13 alkyl derivs., sodium salt (68411-30-3) and possibly others yet to be identified.

[2] In addition to "supporting chemicals", the LAS/ABS Consortium intends to include several "supported chemicals" in its final assessment. These supported chemicals are close structurally-related HPV chemicals (not identifed in the 1990 IUR) that are expected to fit into the LAS/ABS category but for which no additional SIDS endpoint data exist. These include benzenesulfonic acid, (tetrapropenyl)-compd. with 2-propanamine (1:1) (CAS RN 157966-96-6), benzenesulfonic acid, mono-C10-16 alkyl derivs., ammonium salts (CAS RN 68910-31-6), and benzenesulfonic acid, mono-C11-13-branched alkyl derivs., sodium salts (CAS RN 68608-89-9). Inclusion of these chemicals in the final assessment will be dependent upon the degree to which they fit the category defined by the sponsored and supporting HPV chemicals.

assessment as soon as the assessment for the LAB Sulfonic Acid Category has been submitted to the U.S. EPA under the Challenge Program and the assessment for the LAS Category has been submitted to the U.S. EPA for OECD review as part of the ICCA HPV Initiative. It is anticipated that these submissions will occur not later than June 2003 at which time this assessment for LAS/ABS will be completed and submitted to U.S. EPA by the LAS/ABS Consortium.

2.0 Data Collection, Review and Summary

The following steps were followed in the preparation of the assessment.

1) a comprehensive literature search and retrieval of SIDS-endpoint data for the six chemicals using complimentary CIS (Chemical Information Systems) and EU (European Union) data sources,
2) a search and retrieval by the Consortium member companies of previously unpublished ("in-house") SIDS-endpoint data for the six chemicals,
3) a review of all available data and determination of data quality,
4) the contracted preparation of robust study summaries for each of the reviewed studies,
5) the development and justification of a category to support "read-across" as part of the assessment. This includes the data for the six sponsored chemicals, data for chemically related substances, and results of structure-activity relationship (SAR) modelling, particularly for physical-chemical properties.
6) construction of a SIDS data matrix and discussion of data adequacy and/or gaps.

EPA has identified approximately 2800 HPV chemicals to be evaluated in the U.S. HPV Challenge Program. Among those chemicals identified by U.S. EPA are the linear and branched alkyl sulfonates. These chemicals are evaluated in this document. Under the U.S. HPV Challenge Program, the use of chemical categories is encouraged to reduce animal testing and produce economic savings. For the purpose of the U.S. HPV Challenge Program, a chemical category is considered to be a group of substances whose physico-chemical, environmental fate and toxicological properties are observed and/or predicted to be similar, or to follow a predictable pattern, as a result of structural similarities. Instead of obtaining a complete data set for all members of a category, data from individual substances may be used to represent the whole category. In total, the available data, modelling and read across are intended to provide a high quality, screening level hazard characterization for the sponsored HPV chemicals. The screening level information or properties included in the U.S. HPV Challenge Program are listed in Table 2-1. Additional data for Beyond SIDS endpoints (e.g., skin and eye irritation, fish bioconcentration, and terrestrial plant and earthworm toxicity) have also been included in the assessment as they may benefit the overall hazard characterization.

Table 2-1 *HPV Endpoints from OECD Screening Information Data Set (SIDS)*

Physico-chemical Properties

Melting Point (OECD 102)
Boiling Point (OECD 103)
Vapour Pressure (OECD 104)
Partition Coefficient (OECD 107, 117)
Water Solubility (OECD 105, 112)

Environmental Fate

Photodegradation (OECD 113, estimate)
Stability in Water -Abiotic Degradation – Hydrolysis (OECD 111)
Transport between Environmental Compartments (Fugacity)
Ready Biodegradability (OECD 301, 302)

Acute Toxicity

Acute Oral Toxicity (OECD 401, 420, 423. 425) ***OR***
Acute Dermal Toxicity (OECD 402) ***OR***
Acute Inhalation Toxicity (OECD 403)

Repeated Dose/Reproduction

28-Day Repeated Dose (OECD 407, 410, 412) ***OR***
90-Day Repeated Dose (OECD 408, 409, 411, 413) ***OR***
Combined Repeated Dose with Repro/Develop Screening (OECD 422)

Teratology (OECD 414) ***OR***
Two-Generation Reproduction Toxicity (OECD 416) ***OR***
Reproduction/Developmental Toxicity Screening Test (OECD 421) ***OR***
Combined Repeated Dose with Repro/Develop Screening (OECD 422)

Mutagenicity

In-vitro *Bacterial and Non-Bacterial Gene Mutation Assay (OECD 471, 472, 480)* ***OR***
Gene mutation test with mouse lymphoma (OECD 476)

In-vitro *Chromosome Aberration Test with Human Lymphocytes (OECD 473)* ***OR***
Sister Chromatid Exchange Assay (OECD 479)

In-vivo *Mouse Bone Marrow Chromosome Aberration (OECD 475)*[3]

Ecotoxicity

Fish Static Acute Toxicity (OECD 203),
Daphnia Acute (48 Hr -Static) Immobilization Test (OECD 202)
Freshwater algae Growth Inhibition Test (OECD 201)

[3] Other tests to assess chromosomal effects or gene mutations are accepted by the US-EPA (OECD 474, 477-478 and 483-486).

2.1 Public and In-House Records

The literature search employs a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute For Systems, Informatics And Safety (ISIS) ECDIN (Environmental Chemicals Data Information Network) databases. These databases include:

- *Registry of Toxic Effects of Chemical Substances (RTECS)*
- *Toxic Substances Control Act Test Submissions (TSCATS)*
- *Integrated Risk Information System (IRIS)*
- *Chemical Carcinogenesis Research Information (CCRIS)*
- *GENETOX*
- *The Environmental Mutagen Information Center (EMIC)*
- *The Environmental Teratology Information Center (ETIC)*
- *The Developmental and Reproductive Toxicology Database (DART)*
- *The Catalog of Teratogenic Agents (CTA)*
- *ENVIROFATE, DATALOG, AQUIRE, PHYOTOX and TERRATOX*

CAS RNs provided by the Consortium members were used to match records available in each database. Consortium members also provided previously unpublished reports and/or relevant data in their possession. All reports identified were subject to a reliability check for determining adequacy in developing the HPV/SIDS data profile.

2.2 Structure-Activity Relationships

As noted in U.S. HPV Challenge Program guidance, modelled structure-activity relationship results can be used to supplement available data. The Estimations Programs Interface for Windows (EPIWIN) suite of models are available and applied, as warranted, to fill data requirements, particularly in the physico-chemical properties of the sponsored chemicals. The required inputs are the CAS RN or chemical structure in Simplified Molecular Input Line Entry System (SMILES) notation. The estimates from the model are applicable to most organic chemicals.

3.0 Data Reliability

In accordance with U.S. HPV Challenge Program guidance (i.e., Determining Adequacy of Existing Data), data reliability was established following the rules described by Klimisch et al. (1997). The Klimisch scoring system results are presented in the robust study summaries and in the data matrix. Key features for scoring include: test substance identification; Good Laboratory Practices (GLP) vs. non-GLP studies; details of test methodology; and the importance of the availability of statistical analyses for establishing the difference between treatment and control groups. The use of sound scientific judgement is acknowledged as an important principle for assessing data adequacy and reliability. The following four categories of reliability are identified in the Klimisch scoring system. Each study/data point included in this assessment is assigned one of these four scores:

1 **Reliable without Restriction**: Includes studies or data complying with GLP procedures, and/or with valid and/or internationally accepted testing guidelines, or in which the key test parameters are documented and comparable to these guidelines.

2 **Reliable with Restrictions:** Includes studies or data in which key test parameters are documented but vary slightly from test guidelines.

3 **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

4 **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g., listed in abstracts or secondary literature (e.g. reference books) but which generally are considered reliable sources of information.

4.0 Chemical Structure and Composition

Linear (designated "LAS") and non-linear or branched (designated "ABS") alkylbenzene sulfonates are anionic surfactants with molecules characterized by a hydrophobic (apolar) and a hydrophilic (polar) group. As a class of chemicals, they are generally mixtures of closely related isomers and homologues. Each molecule contains an aromatic ring sulfonated at the *para* position and attached to either a linear or a branched alkyl chain at any position except the terminal carbons (Valtorta et al, 2000). Chain lengths vary but are predominantly in the range of C10 to C14. Most commercial LAS/ABS products are mixtures but they can be prepared as pure homologues (e.g., a pure C12). The LAS/ABS chemicals are prepared by sulfonation of linear and non-linear alkylbenzenes. Linear structures of alkylbenzene (sulfonic acid derivatives) are based on the reaction of an alpha olefin (i.e., $R\text{-}CH{=}CH_2$) with benzene, in the presence of sulphuric acid (SO_3), with or without a catalyst. Sodium hydroxide (NaOH) or some other salt is used to neutralize.

Branched alkylbenzene structures (ABS), as depicted in Figure 4-1, can also be prepared by several methods. These include the reaction of propylene ($CH_3CH{:}CH_2$) oligomers with benzene, or $CH_3\text{-}(CH)_{11}\text{-}$ phenol ring, in the presence of sulphuric acid (SO_3), with or without a catalyst. Sodium hydroxide (NaOH) or some other salt is used to neutralize.

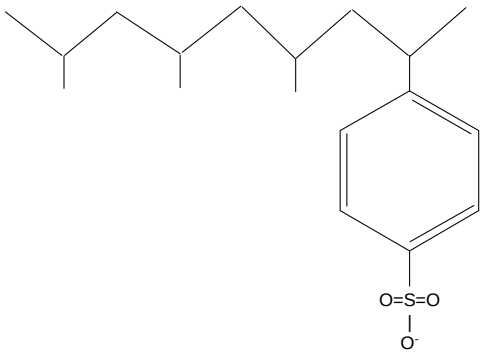
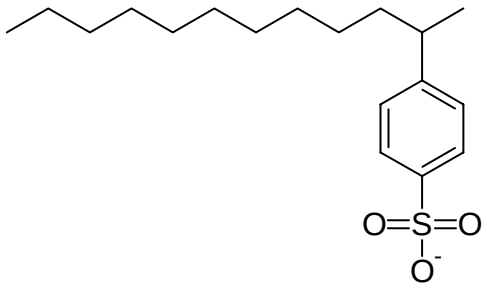


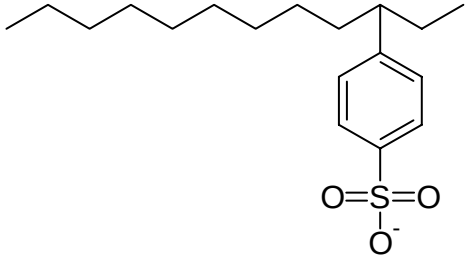
Figure 4-1. Example of structural formula for branched alkyl (here: dodecyl or C12) benzene sulfonates (counter-ion not shown).

Using or not using a catalyst, as well as using different catalysts, will produce different amounts of the 2-, 3-, 4-, 5- and 6-phenyl isomers. The 1-phenyl isomer is not formed. Figure 4-2 shows illustrations of general structures of (in this case a linear) alkylbenzene sulfonate (LAS), with the phenyl ring attached to the 2-, 3- or 4-position of the alkyl chain. Table 4-1 presents the typical composition of the product as a function of the catalyst used during synthesis.

(a)



(b)



(c)

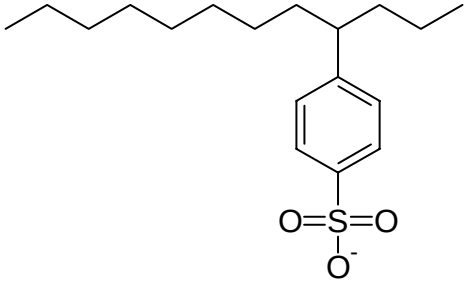


Figure 4-2. General structural formula for (in this case a linear) alkylbenzene sulfonate (counter-ion not shown) with the phenyl ring attached to the (a) 2-position, (b) 3-position and (c) 4-position of the alkyl (here: dodecyl or C12) chain.

Table 4-1 Typical composition of LAS/ABS structures as a function of catalyst

Composition	HF catalysed	$AlCl_3$ catalysed	Fixed bed
1-phenyl	0	0	0
2-phenyl	18.5-22.5%	25-33%	25%
3-phenyl	18.5-25.5%	21-24%	21%
4-phenyl	14.5-30%	13-28%	20%
5-phenyl	0-24.5%	0-23%	18%
6-phenyl	0	0-16.5%	14%

4.1 Sponsored Chemicals

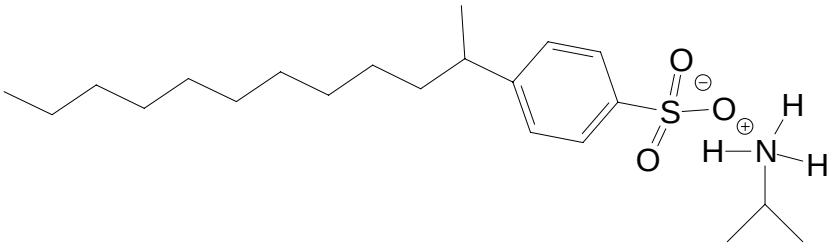
The six HPV chemicals sponsored by the Consortium are depicted below. Chemicals A, B, C are linear (LAS) alkylbenzene sulfonates and chemicals D, E and F are branched (ABS) alkylbenzene sulfonates. It should be noted that, of the several isomeric structures that an LAS/ABS compound can have (see Figure 4.1), only the 2-phenyl isomer is drawn in the representative structure drawings shown below. Also, the commercial LAS/ABS products are mixtures of various alkyl chain lengths, typically from about C10 to C14. Even the compounds named "dodecyl" (=C12) are, in fact, a mixture of alkyl chain lengths. Table 4-2 shows the typical chain length distribution for the linear LAS/ABS substances. The average chain length for the branched LAS/ABS substances is C12.

Table 4-2 Typical chain length distribution of linear LAS/ABS

Chain length	< C10	C10	C11	C12	C13	≥ C14
Amount (%)	≤ 2	≤ 25	~ 40	≥ 25	≤ 15	≤ 2

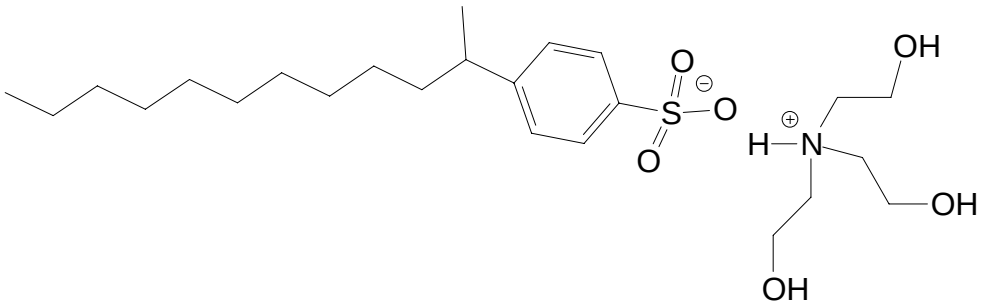
Where C10 + C11 ≥ 50%; and C10 + C11 + C12 ≥ 85%

Substance "A": linear



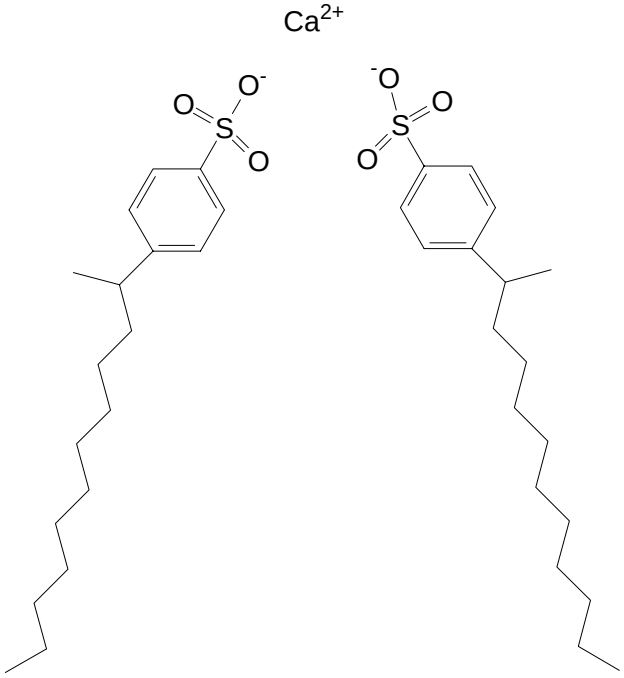
CAS: 26264-05-1, Benzenesulfonic acid, dodecyl-, compd. with 2-propanamine (1:1)
The alkyl chain drawn is C12; the counter-ion (+ charge) is 2-propanamine in a 1:1 molecule ratio.

Substance “B”: linear



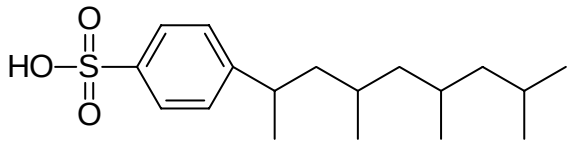
CAS 27323-41-7, Benzenesulfonic acid, dodecyl-, compd. with 2,2’,2’’-nitrilotris(ethanol) (1:1)
The alkyl chain drawn is C12; the counter-ion (+ charge) is 2,2’,2”-nitrilotris(ethanol) in a 1:1 molecule ratio.

Substance "C": linear



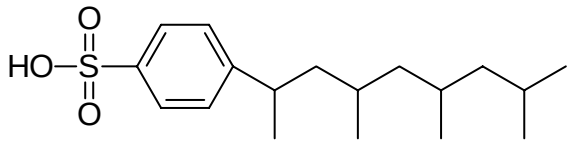
CAS 26264-06-2, Benzenesulfonic acid, dodecyl-, calcium salt
The alkyl chain drawn is C12; the counter-ion (+ charge) is calcium in a 2:1 molecule ratio.

Substance “D”: branched



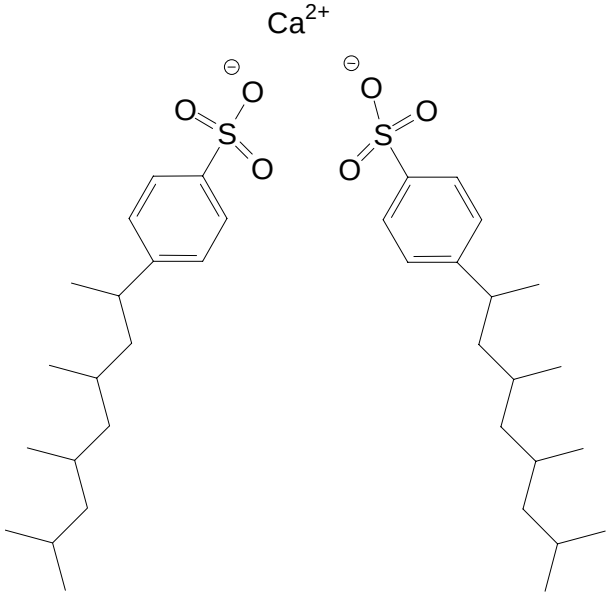
CAS 68411-32-5, Benzenesulfonic acid, dodecyl-, branched
The alkyl chain drawn is C12; there is no counter-ion.

Substance “E”: branched



CAS 68608-88-8, Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.
The alkyl chain drawn is C12; there is no counter-ion.

Substance “F”: branched

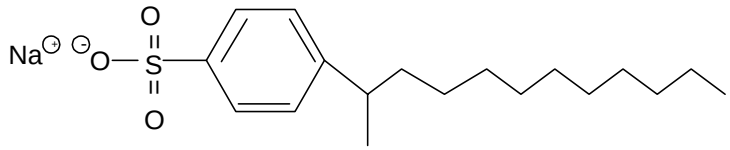


CAS 68953-96-8, Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts
The alkyl chain drawn is C12; the counter-ion (+ charge) is calcium in a 1:2 molecule ratio.

4.2 Supporting Chemicals

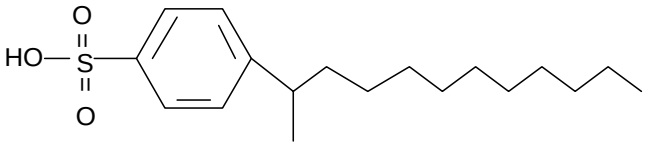
In addition to the six sponsored chemicals, the Consortium has identified several chemicals that are very closely related with regard to their chemical structure and for which there are data for SIDS endpoints that can be used to support the LAS/ABS category. For purposes of this assessment these chemicals are named “Substance 1”, “Substance 2” and “Substance 3”. Their chemical names, CAS registration numbers and representative structures are shown below.

Substance “1”: linear



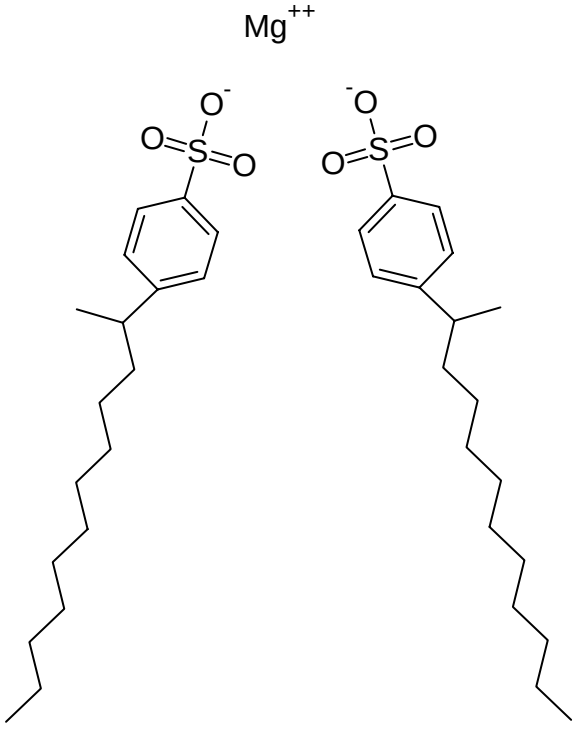
CAS: 68411-30-3, Benzenesulfonic acid, C10-13-alkyl derivs., sodium salt
The alkyl chain drawn is C12; the counter-ion (+ charge) is sodium in a 1:1 molecule ratio.

Substance “2”: linear



CAS: 42615-29-2, Benzenesulfonic acid, linear alkyl
The alkyl chain drawn is C12; there is no counter-ion.

Substance "3": linear



CAS: 68584-26-9, Benzenesulfonic acid, C10-16-alkyl derivs., magnesium salts
The alkyl chain drawn is C12; the counter-ion (+ charge) is magnesium in a 1:2 molecule ratio.

4.3 The LAS/ABS Chemicals as a Category

Chemical categories can be constructed on the basis of similar and/or patterned chemical structures and compositions as well as on similar and/or predictable physico-chemical, environmental fate and toxicological properties. As described previously, the six sponsored chemicals are derived from comparable chemical reactions. The resulting structures are generally mixtures of C10 to C14 linear or mono-branched alkyl chains with a single benzene ring sulfonated at the *para* position attached (at various points) to the alkyl chain. Substances "A" and "B" are ammonium salts, Substances "C" and "F" are calcium salts, and Substances "D" and "E" are acid forms.

In water, all products of acid-base reactions at moderate to low concentrations are essentially completely dissociated into solvated ions. The sulfonic acids and their salts (including Substances "C-F") should dissociate almost completely up to the critical micelle concentration. At or above this point, any additional surfactant exists in micelle form and the counter ions are somewhat associated. The LAS/ABS surfactants will form micelles with an apolar core of alkyl tails and a surface consisting of sulfonate groups, thus rendering the surface negatively charged. The counter ions will be attracted by this negatively charged layer, thereby forming a now positively charged layer around the micelle (electronic double layer). Hence, semi-dissociation is observed for the LAS/ABS substances

in aqueous solution above the critical micelle concentration. The functionalized ammonium cations encountered in Substances “A” and “B” are expected to remain intact in aqueous solutions.

The case for the six sponsored chemicals to be considered a category on the basis of comparable/predictable physico-chemical, environmental fate and toxicological properties will require the evaluation of the available data for these chemicals and for the supporting chemicals. The available data for the sponsored chemicals and for two supporting chemicals is presented in the following pages. The data for the additional supporting chemicals is pending the availability of completed assessments from the Industry Coalition for the SIDS Assessment of LAS and from the LAB Sulfonic Acid Coalition. Some of the members of those two coalitions are also members of the LAS/ABS Consortium and therefore the data and assessment for the LAS Category will become readily available as soon as the two coalitions complete their work (anticipated during the first half of 2003).

5.0 Summary of Endpoints

The available data are indicated for each of the six sponsored chemicals (A-F) and for two supporting chemicals (2 and 3). The corresponding number of the robust study summary is presented in the column marked “Ref”. In addition, the far right column indicates those endpoints for which read across data are known to exist as part of the assessments being prepared by the Industry Coalition for the SIDS Assessment of LAS and by the LAB Sulfonic Acid Coalition. As indicated in the footnotes, these read across data are expected to come from structurally related chemicals that are part of either an HPV submission for a linear alkylbenzene sulfonates category that is in progress and for which the U.S. EPA is the country sponsor at OECD, or a U.S. HPV Challenge submission for linear alkylbenzene sulfonic acids category. These additional data will be added to this assessment once they become available.

5-1 Evaluation Physico-Chemical Endpoints:

Table 5.1

Substance →	**A**	*Ref*	**B**	*Ref*	**C**	*Ref*	**D**	*Ref*	**E**	*Ref*	**F**	*Ref*	Read Across Data including Substance 1 (LAS) [1]
Melting point													√
Boiling point	>149ºC	9.1.01									117ºC	9.1.03	√
Vapour pressure	<3100 Pa	9.1.01									733 Pa	9.1.03	√
Partition coefficient (log Kow)													√
Water solubility	dispersible	9.1.01			dispersible	9.1.02					dispersible	9.1.03	√

[1] Data are in the Assessment Plans and Dossiers under development for the LAS Category and the LAB Sulfonic Acid Category.

5-2 Evaluation Environmental Fate Endpoints:

Table 5.2

Substance →	**A** *Ref*	**B** *Ref*	**C** *Ref*	**D** *Ref*	**E** *Ref*	**F** *Ref*	**2** *Ref*	Read Across Data including Substance 1 (LAS) [1]
Photodegradation								√
Hydrolysis								√
Transport between Environ. Comparts.								Mackay Fugacity
Biodegradation		71% in 28 days 9.2.02		64-73% in 28 days 9.2.03				√
Bioconcentration[2]							BCF = 104 9.2.04	√

[1] Data are in the Assessment Plans and Dossiers under development for the LAS Category and the LAB Sulfonic Acid Category.
[2] A Beyond SIDS endpoint.

5-3 Evaluation Ecotoxicity Endpoints:

Table 5.3

Substance →	**A** *Ref:*	**B** *Ref:*	**C** *Ref:*	**D** *Ref:*	**E** *Ref:*	**F** *Ref.*	**2** *Ref*	Read Across Data including Substance 1 (LAS) [1]
Fish (96h-LC50)	20 mg/L 9.3.01						3.4 – 4.0 mg/L 9.3.26	√
Daphnia (48h-EC50)	2.2 mg/L 9.3.07							√
Algae 72h-EbC50 72h-ErC50								√
Terrestrial Plant (21-day EC50)[2]							167-316 mg/kg 9.3.27	√
Earthworm (14-day LC50)[2]							>1000 mg/kg 9.3.28	√

[1] Data are in the Assessment Plans and Dossiers under development for the LAS Category and the LAB Sulfonic Acid Category.
[2] A Beyond SIDS Endpoint.

5-4 Evaluation Health Effects Endpoints:

Table 5.4

Substance →	**A**	*Ref:*	**B**	*Ref:*	**C**	*Ref:*	**D**	*Ref:*	**E**	*Ref:*	**F**	*Ref:*	**2**	*Ref*	**3**	*Ref*	Read Across Data including Substance 1 (LAS) [1]
Acute oral	1836 mg/kg	9.4.01	1653 mg/kg	9.4.03	1300 mg/kg	9.4.05	1080 mg/kg	9.4.06	520 mg/kg	9.4.07			650 mg/kg	9.4.15			√
	1300 mg/kg	9.4.02	>1953 mg/kg	9.4.04													
Acute dermal			>4199 mg/kg	9.4.16													√
Acute inhalation																	√
Genotoxicity (*in-vivo*)																	√
Genotoxicity (*in-vitro*)													Neg.	9.4.38			√
													Neg.	9.4.39			
Repeat Dose Toxicity			Rabbit 90-day dermal NOAEL >5 mg/kg bw (only dose tested)	9.4.40									Monkey 28-day oral + subcut. NOAEL = 60 mg/kg bw	9.4.42			√
													Mouse 6- mo. drinking water NOAEL < 17 mg/kg (single dose)	9.4.47			

Substance →	**A** *Ref:*	**B** *Ref:*	**C** *Ref:*	**D** *Ref:*	**E** *Ref:*	**F** *Ref:*	**2** *Ref*	**3** *Ref*	Read Across Data including Substance 1 (LAS) [1]
Reproduction / Developmental • Multi-generation		Rat 2-gen. dermal NOAEL >1.5 mg/kg bw (only dose tested) 9.4.48					Mouse embryo incubate NOAEL 0.025% for 1-hr 0.01% for 5-day 9.4.50	Rat 2 gen. dietary NOAEL repro = 222; F2 growth =50 mg/kg bw 9.4.52	√
• Teratology		Rat dermal F0 & F1 NOAEL >10 mg/kg bw (only dose tested) 9.4.53					Ratdermal NOAEL F0=20.1 F1=82 mg/kg bw 9.4.54 **oral** NOAEL rat F0=300 rabbit F0>2<300 mouse F0>2<300 mg/kg bw No terato-tox. at any dose for 3 species 9.4.55 **dermal** NOAEL rat F0=60 rabbit F0=9 mouse F0=50 mg/kg bw No terato-tox. at any dose for 3 species 9.4.56	Rabbit oral NOAEL F0 & F1 = 60 mg/kg bw 9.4.57 Rabbit dermal NOAEL F0 & F1=3% (max. dose) 9.4.58 Rat dermal NOAEL F0 & F1 =7% (max. dose) 9.4.59	√

Substance →	**A** *Ref:*	**B** *Ref:*	**C** *Ref:*	**D** *Ref:*	**E** *Ref:*	**F** *Ref:*	**2** *Ref*	**3** *Ref*	Read Across Data including Substance 1 (LAS) [1]
Irritation[2]									
• skin	Irritating 9.4.21	Irritating 9.4.22	Moderatly Irritating 9.4.23	Irritating 9.4.22	Irritating 9.4.24 Irritating 9.4.25				√
• eye	Irritating 9.4.30		Severely Irritating 9.4.31						√
• sensitization									√

[1] Data are in the Assessment Plans and Dossiers under development for the LAS Category and the LAB Sulfonic Acid Category.
[2] A Beyond SIDS Endpoint.

6.0 Hazard Characterization

Hazard characterization of the six sponsored chemicals, and of the six as a category, will be completed once the data for the additional supporting chemicals become available and can be fully integrated into the assessment. It will include characterization of physico-chemical, environmental fate, ecotoxicology and mammalian toxicity endpoints.

7.0 Data-Gap Analysis

The data-gap analysis for the LAS/ABS Category will be conducted once the data for the additional supporting chemicals become available and can be fully integrated into the assessment.

8.0. References

8.1 References Cited in the Text

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8.2 References for the Robust Study Summaries

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3.	**Harcros**	MSDS and product specification Casul 55HF and Casul 70HF		2000
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5.	**Heywood R., James R., Sortwell R.**	Toxicology studies of linear alkylbenzene sulphonate (LAS) in rhesus monkeys I. Simultaneous oral and subcutaneous administration for 28 days	Toxicol 11: 245-250	1978
6.	**Inoue K., Sunakawa T.**	Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds	Fd Cosmet Toxicol 18: 289-296	1980
7.	**Ishii Y., Samejima Y., Saji F., Nomura T.**	Effect of alcohol sulfonate and natural soap on the development of fertilized eggs of the mouse in vitro	Mut. Res. 242: 151-155	1990

	Author/ Source	Title	Journal/ performing laboratory	Year
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