

## Supporting Documents for Initial Risk-Based Prioritization of High Production Volume Chemicals

### Petroleum Additive Alkaryl Sulfonate Category

#### Sponsored Chemicals

Sulfonic acids, petroleum, calcium salts	(CASRN 61789-86-4)
Sulfonic acids, petroleum, barium salts	(CASRN 61790-48-5)
Sulfonic acids, petroleum, sodium salts	(CASRN 68608-26-4)
Sulfonic acids, petroleum, calcium salts, overbased	(CASRN 68783-96-0)
Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts	(CASRN 70024-69-0)
Benzenesulfonic acid, mono-C15-30-branched alkyl and di-C11-13-branched and linear alkyl derivs., calcium salts, overbased	(CASRN 71486-79-8)
Benzenesulfonic acid, mono-C15-30-branched alkyl and di-C11-13-branched and linear alkyl derivs.	(CASRN 71549-79-6)
Benzenesulfonic acid, mono- and dialkyl derivs., magnesium salts	(CASRN 71786-47-5)
Benzenesulfonic acid, mono- and di-C15-30-alkyl derivs., sodium salts	(CASRN 78330-12-8)
Benzenesulfonic acid, C14-24-branched and linear alkyl derivs., calcium salts	(CASRN 115733-09-0)
Benzenesulfonic acid, C14-24-branched and linear alkyl derivs., calcium salts, overbased	(CASRN 115733-10-3)
Benzenesulfonic acid, C14-24-branched and linear alkyl derivs.	(CASRN 115829-36-2)

#### Supporting Chemicals

Magnesium long chain alkaryl sulfonate (no CASRN)  
C20-24-Alkaryl calcium salt derivative (no CASRN)  
C15-21-Alkaryl calcium salt derivative (no CASRN)

#### Contents:

- Page 2: Background
- Page 4: Screening-Level Risk Characterization: August 2008
- Page 9: Screening-Level Hazard Characterization: August 2008
- Page 31: Screening-Level Exposure Characterization: August 2008

## BACKGROUND

Screening-level hazard, exposure and risk characterizations for high production volume chemicals (HPV) are important contributions to the chemicals cooperation work being done in North America<sup>1</sup> through the EPA Chemical Assessment and Management Program (ChAMP)<sup>2</sup>. These screening-level characterizations are developed by EPA for individual chemicals or chemical categories to support initial Risk-Based Prioritizations (RBPs) for HPV chemicals. These screening-level characterizations are technical documents intended primarily to inform the Agency's internal decision-making process. Accordingly, they are written for assessment professionals and assume a degree of technical understanding. Each of the support documents is described below.

The Risk-Based Prioritizations are found in an accompanying document and are written for a general audience. They present EPA's initial thinking regarding the potential risks presented by these chemicals and future possible actions that may be needed.

### Hazard Characterizations for HPV Chemicals

EPA's screening-level hazard characterizations are based primarily on the review of the summaries of studies and other information submitted by the chemical sponsor(s) under the HPV Challenge Program<sup>3</sup>. These studies included in the scope of the HPV Challenge comprise the Screening Information Data Set (SIDS) of the Organization for Economic Cooperation and Development (OECD)<sup>4</sup>, an internationally recognized battery of tests that provides the basic data necessary to make an initial evaluation of a chemical's hazards and fate. In preparing the initial hazard characterizations, EPA also consulted a variety of reliable sources<sup>5</sup> for additional relevant information and considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of an HPV submission, EPA also searched publicly available databases<sup>6</sup> for information entered from one year prior to the HPV submission through May 2008. The screening-level hazard characterization is performed according to established EPA guidance<sup>7</sup>. A more detailed description of the hazard characterization process is available on the EPA website<sup>8</sup>.

With respect to chemicals for which internationally-accepted OECD SIDS Initial Assessment Profiles (SIAP) and Initial Assessment Reports (SIAR) were available, EPA did not generate its own screening-level hazard characterization, but did check for and incorporate updated information in the risk characterization.

### Exposure Characterizations for HPV Chemicals

EPA recently received exposure-related data on chemicals submitted in accordance with the requirements of Inventory Update Reporting (IUR)<sup>9</sup>. The 2006 IUR submissions pertain to chemicals manufactured in

---

<sup>1</sup> U.S. EPA – U.S. Commitments to North American Chemicals Cooperation: <http://www.epa.gov/hpv/pubs/general/sppframework.htm>.

<sup>2</sup> U.S. EPA – ChAMP information: <http://www.epa.gov/champ/>.

<sup>3</sup> U.S. EPA – HPV Challenge Program information: <http://www.epa.gov/hpv>.

<sup>4</sup> U.S. EPA – Technical Guidance Document, OECD SIDS Manual Sections 3.4 and 3.5: <http://www.epa.gov/chemrtk/pubs/general/sidsappb.htm>.

<sup>5</sup> U.S. EPA – Public Database Hazard Information: <http://www.epa.gov/hpvis/hazardinfo.htm>.

<sup>6</sup> U.S. EPA – Public Database Update Information: <http://www.epa.gov/chemrtk/hpvis/updateinfo.htm>.

<sup>7</sup> U.S. EPA – Risk Assessment Guidelines: <http://cfpub.epa.gov/ncea/raf/rafguid.cfm>.

<sup>8</sup> U.S. EPA – About HPV Chemical Hazard Characterizations: <http://www.epa.gov/hpvis/abouthc.htm>.

<sup>9</sup> U.S. EPA – Basic IUR Information: <http://www.epa.gov/opptintr/iur/pubs/guidance/basic-information.htm>.

(including imported into) the U.S. during calendar year 2005 in quantities of 25,000 pounds or more at a single site. The reports include the identity, the quantity, and the physical form of the chemical manufactured or imported, and the number of workers reasonably likely to be exposed during manufacture of the chemical. For chemicals manufactured or imported in quantities of 300,000 pounds or more at a single site, additional reported information includes: the industrial processing and uses of the chemical; the number of industrial processing sites and workers reasonably likely to be exposed to the chemical at those sites; the consumer and commercial uses of the chemical; and an indication whether the chemical was used in products intended for use by children under 14 years of age.

EPA's screening-level exposure characterizations are based largely on the information submitted under the IUR reporting, although other exposure information submitted to the Agency (for example, in HPV submissions) or readily available through a limited set of publicly accessible databases<sup>10</sup> was also considered. The screening-level Exposure Characterizations identify a potential (high, medium, or low) that each of five populations – the environment, the general population, workers, consumers, and children – might be exposed to the chemical. In most cases, this potential doesn't address the quantity, frequency, or duration of exposure, but refers only to the likelihood that an exposure could occur.

In many instances EPA is not able to fully disclose to the public all the IUR exposure-related data reviewed or relied upon in the development of the screening-level documents because some of the material was claimed as confidential business information (CBI) when it was submitted to the Agency. These CBI claims do limit the Agency's ability to be completely transparent in presenting some underlying exposure and use data for chemicals in public documents. EPA does consider all data, including data considered to be CBI, in the screening-level exposure and risk characterization process, and endeavors whenever possible to broadly characterize supporting materials claimed as confidential in ways that do not disclose actual CBI.

### **Risk Characterizations for HPV Chemicals**

EPA combines the information from the screening-level exposure characterization with the screening-level hazard characterization to develop a qualitative screening-level risk characterization, as described in the Agency's guidance on drafting risk characterizations<sup>11</sup>. These screening-level risk characterizations are technical documents intended to support subsequent priority-setting decisions and actions by OPPT. The purpose of the qualitative screening-level risk characterization is two-fold: to support initial risk-based decisions to prioritize chemicals, identify potential concerns, and inform risk management options; and to identify data needs for individual chemicals or chemical categories.

These initial characterization and prioritization documents do not constitute a final Agency determination as to risk, nor do they determine whether sufficient data are available to characterize risk. Recommended actions reflect EPA's relative judgment regarding this chemical or chemical category in comparison with others evaluated under this program, as well as the uncertainties presented by gaps that may exist in the available data.

---

<sup>10</sup> U.S. EPA – Summary of Public Databases Routinely Searched: <http://www.epa.gov/chemrtk/hpvis/pubdtsum.htm>.

<sup>11</sup> U.S. EPA – Risk Characterization Program: <http://www.epa.gov/osa/spc/2riskchr.htm>.

**QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION  
OF HIGH PRODUCTION VOLUME CHEMICALS**

**CHEMICAL CATEGORY NAME  
Petroleum Additive Alkaryl Sulfonate**

**SPONSORED CHEMICALS**

<b>Sulfonic acids, petroleum, calcium salts</b>	<b>CAS No. 61789-86-4</b>
<b>Sulfonic acids, petroleum, barium salts</b>	<b>CAS No. 61790-48-5</b>
<b>Sulfonic acids, petroleum, sodium salts</b>	<b>CAS No. 68608-26-4</b>
<b>Sulfonic acids, petroleum, calcium salts, overbased</b>	<b>CAS No. 68783-96-0</b>
<b>Benzenesulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub> alkyl derivatives, calcium salts</b>	<b>CAS No. 70024-69-0</b>
<b>Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased</b>	<b>CAS No. 71486-79-8</b>
<b>Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives</b>	<b>CAS No. 71549-79-6</b>
<b>Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts</b>	<b>CAS No. 71786-47-5</b>
<b>Benzenesulfonic acid, C<sub>15</sub>-C<sub>30</sub> alkyl derivatives, sodium salts</b>	<b>CAS No. 78330-12-8</b>
<b>Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts</b>	<b>CAS No. 115733-09-0</b>
<b>Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased</b>	<b>CAS No. 115733-10-3</b>
<b>Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alky derivatives</b>	<b>CAS No. 115829-36-2</b>

**SUPPORTING CHEMICALS**

**Magnesium long chain alkaryl sulfonate (no CAS No.)**  
**C<sub>20</sub>-C<sub>24</sub> Alkaryl calcium salt derivative (no CAS No.)**  
**C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative (no CAS No.)**

**August 2008**

**Prepared by**

Risk Assessment Division  
Economics, Exposure and Technology Division  
Office of Pollution Prevention and Toxics  
Environmental Protection Agency  
1200 Pennsylvania Avenue, NW  
Washington, DC 20460-0001

## QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION FOR Petroleum Additive Alkaryl Sulfonate Category

### 1. Category Justification

The 12 members of the Petroleum Additive Alkaryl Sulfonate category are complex mixtures designated as Class 2 substances for TSCA Inventory Reporting. Class 2 substances, in general, have a complex and variable composition depending on their source or methods of derivation. The sulfonated alkylbenzenes are manufactured by the sulfonation of either synthetic alkylbenzene substrates or naturally occurring alkylaromatic-rich fractions of heavy lubricating oil base stocks derived from petroleum streams. The alkyl substituent group may vary in number (e.g., mono- or dialkyl), position (e.g., predominantly meta or para to the sulfonic acid position), chain length (e.g., C<sub>14</sub> to C<sub>30</sub>) or in the degree of branching. Branched and linear alkyl groups of 20 or more carbons are used to enhance oil solubility. The sponsor grouped the chemicals based on the similarities in structure, physical-chemical properties, environmental fate, aquatic and mammalian toxicity. EPA considered this grouping acceptable for the purposes of the HPV Challenge Program and further accepts this category for prioritization in the Chemical Assessment and Management Program (ChAMP).

### 2. Physical-Chemical Properties and Environmental Fate

Members of the alkaryl sulfonate category are dark-colored viscous liquids in the presence of a manufacturing diluent and solids at room temperature if diluent is absent. All substances in this category have negligible vapor pressure. Volatilization is also negligible because ionic substances do not volatilize. Water solubility is negligible, but alkaryl sulfonates are considered water dispersible. They are expected to be stable to hydrolysis. All substances in the alkaryl sulfonate category are judged to be minimally mobile in soil. In the atmosphere, the alkaryl sulfonates exist primarily in the particulate phase, and vapor phase photooxidation is negligible. Estimated BCF values suggest that the potential for alkaryl sulfonates to bioaccumulate is low (B1). Measured biodegradation data for several members of this category indicate that alkaryl sulfonates are not readily biodegradable. Overall, the environmental persistence potential of these substances is expected to be moderate (P2).

### 3. Hazard Characterization

*Aquatic Organism Toxicity.* All aquatic toxicity studies submitted were conducted using Water Accommodated Fractions (WAFs). For all but one algae study, no acute toxicity occurred at any of the loading rates. EPA therefore concludes, based on the weight of evidence, that no acute effects are expected at saturation and that acute toxicity to aquatic organisms is low. Although the weight of evidence indicates the acute toxicity of these chemicals is low, their potential dispersibility and persistence suggest that there may be potential for toxicity to occur to aquatic organisms under chronic exposure conditions.

*Human Health Toxicity.* The acute oral toxicity for the members of this category is low. Members of the category and supporting chemicals caused irritation and point of entry effects with repeated exposures via the oral, dermal and inhalation routes. Systemic toxicity is low in the oral and dermal repeated-dose studies of rats with several category chemicals and a supporting chemical. One inhalation repeated-dose rat study of one category member showed moderate respiratory tract irritation and inflammation. A one generation study of one category member showed there were no treatment-related effects on the parents or offspring for the reproductive or developmental toxicity endpoints. None of the genetic toxicity tests of the category members or supporting chemicals showed increased gene mutations or chromosomal aberrations.

#### **4. Exposure Characterization**

The alkaryl sulfonate category chemicals have an aggregated production and/or import volume in the range of 36 million to 211 million pounds. The aggregated production volume includes 11 of the 12 chemicals in the category and excludes benzenesulfonic acid, mono-C16-24-alkyl derives, calcium salt (CAS# 70024-69-0), which does not have Inventory Update Reporting (IUR) submissions. Non-confidential IUR information for many of the chemicals in the alkaryl sulfonate category indicates that these chemicals are used as lubricants in the manufacturing and preparation of other chemical products. Nine of the 12 chemicals in this category have IUR submissions that indicate uses in commercial settings or consumer uses.

According to the High Production Volume (HPV) Program submission, alkaryl sulfonates are used as petroleum additives in petroleum base stocks. Petroleum additive alkaryl sulfonates are used to formulate finished lubricating oils including all types of automotive and diesel engine crankcase oils, air and water-cooled two-cycle engine oils, industrial oils, hydraulic fluids, gear oils and metal working lubricating oils. They are used as high temperature detergents to reduce deposits on pistons, engine crankcases, and hydraulic equipment parts and as rust inhibitors during industrial oil use.

*Potential Exposures to the General Population and the Environment:* Based on the use information from the IUR and HPV submissions there is potential for environmental releases to various media including air, water and land. Based on the totality of the information considered, especially IUR information indicating most of these chemicals are not site-limited, EPA identifies, for the purposes of risk-based prioritization, a medium potential for exposure to the general population and the environment.

Persistence and bioaccumulation ratings for the alkaryl sulfonate category chemicals are P2 and B1. These ratings suggest that this category of chemicals is moderately persistent in the environment and is not bioaccumulative.

*Potential Exposures to Workers:* Based on the totality of the information considered, including IUR data and information from the HPV submission, and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for the potential worker exposure. This relative ranking is based on uses that may result in significant inhalation exposure and widespread dermal exposures. These uses

include use in engine oils, metal working, and applications claimed to be confidential under IUR. Alkaryl sulfonate chemicals do not have OSHA Permissible Exposure Limits (PELs).

*Potential Exposures to Consumers:* EPA identifies, for the purposes of risk-based prioritization, a high potential for exposures to consumers from products containing these chemicals. Nine of the twelve chemicals have IUR submissions that indicate uses in commercial settings or consumer uses. Based on non-confidential IUR data, the commercial and consumer uses are lubricants, greases and fuel additives.

*Potential Exposures to Children:* EPA identifies, for the purpose of risk-based prioritization, a medium potential for exposures to children. No uses in products intended for children were reported in the IUR, nor were any found in other data sources. Exposures to children, however, may be expected to occur through the household use of some consumer products.

## 5. Risk Characterization

The statements and rationale provided below are intended solely for the purpose of this screening-level and qualitative risk characterization and will be used for prioritizing substances for future work in the Chemical Assessment and Management Program (ChAMP).

### **Risk Statement and Rationale**

*Potential Risk to Aquatic Organisms from Environmental Releases (LOW CONCERN).* EPA identifies a medium potential for exposure to aquatic organisms from environmental releases. A low acute aquatic hazard considered in combination with the environmental fate characteristics of moderate persistence and low bioaccumulation suggest a low concern for potential acute risk to aquatic organisms from environmental releases.

*Potential Risk to the General Population from Environmental Releases (LOW CONCERN).* EPA identifies a medium potential for exposure to the general population from environmental releases. The potential human health hazard is expected to be low due to the lack of specific toxicity to animals following exposure to high doses. The low hazard and the environmental fate characteristics of moderate persistence and low bioaccumulation suggest a low concern for potential risk to the general population from environmental releases.

*Potential Risk to Workers (LOW CONCERN).* EPA identifies a high relative ranking for potential worker exposure. Overall, the potential health hazard of the alkaryl sulfonate category members is low. The moderate respiratory tract irritation and inflammation seen in one rat study on one category member presents a potential concern for workers exposed to aerosols using metal working lubricating oils. There is also the potential for skin irritation at high concentrations. There are no OSHA PELs for the chemicals in this category. Therefore, taken together, the available information suggests a low overall concern for potential risks to workers with a medium concern for irritation to workers exposed to aerosols via inhalation.

*Potential Risk to Consumers from Known Uses (LOW CONCERN).* EPA identifies a high potential for exposures to consumers from products containing these chemicals. The potential human health hazard is expected to be low due to the lack of specific toxicity to animals following exposure to high doses. Therefore, taken together, the available information suggests a low concern for potential risks to consumers.

*Potential Risk to Children (LOW CONCERN).* EPA identifies a medium potential for exposures to children. The potential human health hazard is expected to be low due to the lack of specific toxicity to young animals following exposure to high doses. Therefore, taken together, the available information suggests a low concern for potential risks to children.



**SCREENING-LEVEL HAZARD CHARACTERIZATION  
OF HIGH PRODUCTION VOLUME CHEMICALS**

**CHEMICAL CATEGORY NAME  
Petroleum Additive Alkaryl Sulfonate**

**SPONSORED CHEMICALS**

<b>Sulfonic acids, petroleum, calcium salts</b>	<b>CAS No. 61789-86-4</b>
<b>Sulfonic acids, petroleum, barium salts</b>	<b>CAS No. 61790-48-5</b>
<b>Sulfonic acids, petroleum, sodium salts</b>	<b>CAS No. 68608-26-4</b>
<b>Sulfonic acids, petroleum, calcium salts, overbased</b>	<b>CAS No. 68783-96-0</b>
<b>Benzenesulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub> alkyl derivatives, calcium salts</b>	<b>CAS No. 70024-69-0</b>
<b>Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased</b>	<b>CAS No. 71486-79-8</b>
<b>Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives</b>	<b>CAS No. 71549-79-6</b>
<b>Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts</b>	<b>CAS No. 71786-47-5</b>
<b>Benzenesulfonic acid, C<sub>15</sub>-C<sub>30</sub> alkyl derivatives, sodium salts</b>	<b>CAS No. 78330-12-8</b>
<b>Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts</b>	<b>CAS No. 115733-09-0</b>
<b>Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased</b>	<b>CAS No. 115733-10-3</b>
<b>Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives</b>	<b>CAS No. 115829-36-2</b>

**SUPPORTING CHEMICALS**

**Magnesium long chain alkaryl sulfonate (no CAS No.)**  
**C<sub>20</sub>-C<sub>24</sub> Alkaryl calcium salt derivative (no CAS No.)**  
**C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative (no CAS No.)**

**August 2008**

**Prepared by**

Risk Assessment Division  
Economics, Exposure and Technology Division  
Office of Pollution Prevention and Toxics  
Environmental Protection Agency  
1200 Pennsylvania Avenue, NW  
Washington, DC 20460-0001

## SCREENING-LEVEL HAZARD CHARACTERIZATION Petroleum Additive Alkaryl Sulfonate Category

### Introduction

The sponsor, The American Chemistry Council Petroleum Additives Panel, Health, Environmental and Regulatory Task Group (HERTG), submitted a Test Plan and Robust Summaries to EPA for the Petroleum Additive Alkaryl Sulfonate Category on October 8, 2001. EPA posted the submission on the ChemRTK Web site on November 30, 2001 (<http://www.epa.gov/chemrtk/pubs/summaries/alklsulf/c13206tc.htm>). EPA comments on the original submission were posted to the website on June 7, 2002. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on June 28, 2002 and October 13, 2005 which were posted to the ChemRTK website on July 23, 2002 and November 30, 2005 respectively. The petroleum additive alkaryl sulfonate category consists of the following chemicals:

#### Sponsored Chemicals

Sulfonic acids, petroleum, calcium salts	CAS No. 61789-86-4
Sulfonic acids, petroleum, barium salts	CAS No. 61790-48-5
Sulfonic acids, petroleum, sodium salts	CAS No. 68608-26-4
Sulfonic acids, petroleum, calcium salts, overbased	CAS No. 68783-96-0
Benzenesulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> alkyl derivatives, calcium salts	CAS No. 70024-69-0
Benzenesulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased	CAS No. 71486-79-8
Benzenesulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives	CAS No. 71549-79-6
Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts	CAS No. 71786-47-5
Benzenesulfonic acid, C <sub>15</sub> -C <sub>30</sub> alkyl derivatives, sodium salts	CAS No. 78330-12-8
Benzenesulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts	CAS No. 115733-09-0
Benzenesulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased	CAS No. 115733-10-3
Benzenesulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives	CAS No. 115829-36-2

#### Supporting Chemicals

Magnesium long chain alkaryl sulfonate	no CAS No.
C <sub>20</sub> -C <sub>24</sub> Alkaryl calcium salt derivative	no CAS No.
C <sub>15</sub> -C <sub>21</sub> Alkaryl calcium salt derivative	no CAS No.
Benzenesulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> -alkyl derivatives, calcium salts	no CAS No.

This screening-level hazard characterization is based primarily on the review of the test plan and robust summaries of studies submitted by the sponsor(s) under the HPV Challenge Program. In preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from 2004 to June 2008: the NLM databases (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, ATSDR, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. Structures of the sponsored chemicals and supporting chemicals are included in the appendix. The screening-level hazard characterization for environmental and human health toxicity is based largely on SIDS endpoints and is described according to established EPA or OECD effect level definitions and hazard assessment practices.

**Category Justification**

The 12 members of the Petroleum Additive Alkaryl Sulfonate category are complex mixtures designated as Class 2 substances for TSCA Inventory Reporting. Class 2 substances, in general, have a complex and variable composition depending on their source or methods of derivation. The sulfonated alkylbenzenes are manufactured by the sulfonation of either synthetic alkylbenzene substrates or naturally occurring alkylaromatic-rich fractions of heavy lubricating oil base stocks derived from petroleum streams. The alkyl substituent group may vary in number (e.g., mono- or dialkyl), position (e.g., predominantly meta or para to the sulfonic acid position), chain length (e.g., C<sub>14</sub> to C<sub>30</sub>) or in the degree of branching. Branched and linear alkyl groups of 20 or more carbons are used to enhance oil solubility. Although branched alkyl groups are generally presumed to be more water-soluble than straight chains, petroleum additive alkaryl sulfonates have very low water solubility and the degree of branching does not affect their solubility and performance in petroleum base stocks. The category members are manufactured in highly refined lubricating base oil, and thus are never isolated. They are used as petroleum additives in petroleum base stocks and sold to oil blenders in packages of concentration from 0.1 to 50 wt. %. The additive packages are blended into finished oils where the typical concentration of the category members ranges from 0.1 to 10 wt. %. The sponsor grouped the chemicals based on the similarities in structure, physical-chemical properties, environmental fate, aquatic and mammalian toxicity.

In its revised submission, in response to EPA comments, the sponsor clarified the identification of the sponsored substances by including structures for each CAS number (see Appendix) and describing the average chain lengths. Typical compositions are characterized by the identification of the presence of branched or linear alkyl groups and the average chain length. The percent composition or identity of the lubricating base oil has not been described. However, given that it is associated with each category member, it is assumed that its contribution to toxicity will be similar to all category members, which is supported by the submitted data. It is still not clear in the test plan if the data submitted are for the commercial product (including the lubricating base oil) or the discrete substance. Given the complexity of the mixtures identified by the CAS numbers, the significance of this discrepancy in the test plan is difficult to determine. However, the robust summaries do reference the test plan when referring to the test substance identification and so EPA agrees with the sponsor's category approach. EPA had requested that for human health, the sponsor expand the discussion in the test plan to address the potential influence of the structural variability (branched versus linear) of the alkyl side-chains of the category members on toxicity. This was particularly relevant to support the use of data from one category member to characterize the toxicity for other category members for the reproductive and developmental toxicity endpoints. This issue was not addressed adequately in the revised test plan.

**Supporting Chemicals Justification**

The sponsor submitted data for additional chemicals to support characterization of some environmental fate (biodegradation) and human health endpoints (acute toxicity and gene mutations). The supporting chemicals are magnesium long chain alkaryl sulfonate (no CAS No.), C<sub>20</sub>-C<sub>24</sub> alkaryl calcium salt derivative (no CAS No.), C<sub>15</sub>-C<sub>21</sub> alkaryl calcium salt derivative (no CAS No.) and benzenesulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub>-alkyl derivatives, calcium salts (no CAS No.). EPA agrees that these are appropriate analogs for the category members.

<u>Supporting Chemicals</u>	<u>CAS No.</u>	<u>Endpoint(s) Supporting</u>
Magnesium long chain alkaryl sulfonate	no CAS No.	Biodegradation
C <sub>20</sub> -C <sub>24</sub> Alkaryl calcium salt derivative	no CAS No.	Biodegradation; Acute toxicity; Genetic toxicity; Repeated-dose toxicity
C <sub>15</sub> -C <sub>21</sub> Alkaryl calcium salt derivative	no CAS No.	Genetic toxicity
Benzenesulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> -alkyl derivatives, calcium salts	no CAS No.	Biodegradation; Acute toxicity to fish

### **Hazard Characterization**

Members of the alkaryl sulfonate category are dark-colored viscous liquids in the presence of a manufacturing diluent and solids at room temperature if diluent is absent. All substances in this category have negligible vapor pressure. Volatilization is also negligible because ionic substances do not volatilize. Water solubility is negligible, but alkaryl sulfonates are considered water dispersible. They are expected to be stable to hydrolysis. All substances in the alkaryl sulfonate category are judged to be minimally mobile in soil. In the atmosphere, the alkaryl sulfonates exist primarily in the particulate phase, and vapor phase photooxidation is negligible. Estimated BCF values suggest that the potential for alkaryl sulfonates to bioaccumulate is low (B1). Measured biodegradation data for several members of this category indicate that alkaryl sulfonates are not readily biodegradable. Overall, the environmental persistence potential of these substances is expected to be moderate (P2).

All aquatic toxicity studies submitted were conducted using Water Accommodated Fractions (WAFs). For all but one algae study, no acute toxicity occurred at any of the loading rates. Based on the overall weight of evidence, EPA therefore concludes that acute effects are not expected at saturation and that acute toxicity to aquatic organisms is low.

The acute oral toxicity for the members of this category is low. Members of the category and supporting chemicals caused irritation and point of entry effects with repeated exposures via the oral, dermal and inhalation routes. Systemic toxicity is low in the oral and dermal repeat-dose studies of rats with several category chemicals and a supporting chemical. One inhalation repeated-dose rat study of one category member showed moderate respiratory tract irritation and inflammation. A one generation study of one category member showed no treatment-related effects on the parents or offspring for the reproductive or developmental toxicity endpoints. None of the genetic toxicity tests of the category members or supporting chemicals showed increased gene mutations or chromosomal aberrations.

Chronic aquatic toxicity remains a data gap under the HPV Challenge Program.

### **1. Physical-Chemical Properties and Environmental Fate**

The physical-chemical properties of members of the alkaryl sulfonate category are summarized in Table 1a, while their environmental fate properties are given in Table 1b. The structures of the compounds are provided in the Appendix.

#### ***Physical-Chemical Properties Characterization***

Substances in the alkaryl sulfonate category are dark-colored viscous liquids in the presence of a petroleum diluent used in manufacturing. If this diluent is absent or removed, alkaryl sulfonates are solids at room temperature. All members of this category have negligible vapor pressure. Water solubility is also negligible, but alkaryl sulfonates form emulsions in water and for this reason are considered water dispersible.

#### ***Environmental Fate Characterization***

Alkaryl sulfonates are expected to partition primarily to soil and sediment, according to the results of a Level III fugacity model that assumes equal emissions to air, water, and soil. All substances in the alkaryl sulfonate category are judged to be minimally mobile in soil. They are expected to undergo negligible hydrolysis. Volatilization is negligible because ionic substances do not volatilize. In the atmosphere, the alkaryl sulfonates exist primarily in the particulate phase, making vapor phase photooxidation negligible. Analysis of 694 ionic compounds, including 37 sulfonic acids and their salts, suggests that these compounds generally have  $\log BCF \leq 2$ <sup>12</sup>. For this reason, the potential for alkaryl sulfonates to bioaccumulate is judged to be low (B1). Biodegradability is expected to vary substantially depending on the degree of alkyl branching. However, measured biodegradation data for several

---

<sup>12</sup>Meylan WM, Howard PH, Boethling RS, Aronson D, Printup H, Gouchie S. 1999. Improved method for estimating bioconcentration/bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4):664-672.

members of this category indicate that alkaryl sulfonates are not readily biodegradable. Overall, the environmental persistence potential of these substances is expected to be moderate (P2).

**Conclusion:** Members of the alkaryl sulfonate category are dark-colored viscous liquids in the presence of a manufacturing diluent and solids at room temperature if diluent is absent. All substances in this category have negligible vapor pressure. Volatilization is also negligible because ionic substances do not volatilize. Water solubility is negligible, but alkaryl sulfonates are considered water dispersible. They are expected to be stable to hydrolysis. All substances in the alkaryl sulfonate category are judged to be minimally mobile in soil. In the atmosphere, the alkaryl sulfonates exist primarily in the particulate phase, and vapor phase photooxidation is negligible. Estimated BCF values suggest that the potential for alkaryl sulfonates to bioaccumulate is low (B1). Measured biodegradation data for several members of this category indicate that alkaryl sulfonates are not readily biodegradable. Overall, the environmental persistence potential of these substances is expected to be moderate (P2).

<b>Property</b>	<b>Sulfonic acids, petroleum, calcium salts</b>	<b>Sulfonic acids, petroleum, barium salts</b>	<b>Sulfonic acids, petroleum, sodium salts</b>	<b>Sulfonic acids, petroleum, calcium salts, overbased</b>	<b>Benzene sulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub> alkyl derivatives, calcium salts</b>	<b>Benzene sulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased</b>	<b>Benzene sulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alky1 and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives</b>	<b>Benzene sulfonic acid, mono- and dialkyl derivatives, magnesium salts</b>	<b>Benzene sulfonic acid, C<sub>15</sub>-C<sub>30</sub> alkyl derivatives, sodium salts</b>	<b>Benzene sulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts</b>	<b>Benzene sulfonic Acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased</b>	<b>Benzene sulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives</b>
CAS No.	61789-86-4	61790-48-5	68608-26-4	68783-96-0	70024-69-0	71486-79-8	71549-79-6	71786-47-5	78330-12-8	115733-09-0	115733-10-3	115829-36-2
Molecular Weight <sup>2</sup>	393-617	490-714	376-600	393-617	421-533	407-617	368-578	461-517	390-600	393-533	393-533	354-494
Physical State	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid	Solid or dark-colored viscous liquid
Melting Point <sup>3</sup>	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data
Boiling Point <sup>3</sup>	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data
Vapor Pressure <sup>3</sup>	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data
Water Solubility	<b>0.402 mg/L at 20°C (measured)</b>	<b>&lt; 1.03 mg/L at 20°C (measured)</b>	<b>≤ 6.38 mg/L at 20°C (measured)</b>	Dispersible	<b>&lt; 0.100 mg/L (measured)</b>	Dispersible	<b>0.075 mg/L (measured)</b>	Dispersible	<b>38.2 mg/L at 20°C (measured)</b>	<b>0.479 mg/L at 20°C (measured)</b>	Dispersible	0.02 mg/L at 25°C (estimated) <sup>4,5</sup>
Log K <sub>ow</sub>	No data <sup>6</sup>	No data <sup>6</sup>	7.5 (estimated) <sup>4,5</sup>	No data <sup>6</sup>	<b>&gt; 6.0 (measured)</b>	No data <sup>6</sup>	<b>&gt; 6.7 (measured)</b>	3.3 (estimated) <sup>4,5</sup>	6.3 (estimated) <sup>4,5</sup>	No data <sup>6</sup>	No data <sup>6</sup>	7.2 (estimated) <sup>4,5</sup>

<sup>1</sup>American Chemistry Council; Petroleum Additives Panel; Health, Environmental, and Regulatory Task Group. 2005. Revised Robust Summary and Test Plan for Alkaryl Sulfonate Category.

<http://www.epa.gov/chemrtk/pubs/summaries/alklsulf/c13206tc.htm>.

<sup>2</sup>Equivalent weight; molecular weight of one alkylbenzene sulfonic acid plus molecular weight of metal.

<sup>3</sup>These complex mixtures will not have a well-defined melting point, boiling point, or vapor pressure. De-oiled petroleum additive alkaryl sulfonates are solid.

<sup>4</sup>USEPA. 2008. Estimation Programs Interface Suite™ for Microsoft® Windows, v3.20. United States Environmental Protection Agency, Washington, DC, USA.

<http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>.

<sup>5</sup>Data not provided in test plan or robust summary; estimated by EPA using a representative structure.

<sup>6</sup>Estimated value is greater than the range (-4 to 10) where KOWWIN v. 1.66 estimates a have been shown to be valid. It is reasonable to conclude that this prediction is indicative that the log Kow for this chemical is high (> 4).

Table 1b. Environmental Fate Properties of Alkaryl Sulfonate Category<sup>1</sup>

Property	Sulfonic acids, petroleum, calcium salts	Sulfonic acids, petroleum, barium salts	Sulfonic acids, petroleum, sodium salts	Sulfonic acids, petroleum, calcium salts, overbased	Benzene sulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> alkyl derivatives, calcium salts	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives	Benzene sulfonic acid, mono- and dialkyl derivatives, magnesium salts	Benzene sulfonic acid, C <sub>15</sub> -C <sub>30</sub> alkyl derivatives, sodium salts	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts	Benzene sulfonic Acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives
CAS No.	61789-86-4	61790-48-5	68608-26-4	68783-96-0	70024-69-0	71486-79-8	71549-79-6	71786-47-5	78330-12-8	115733-09-0	115733-10-3	115829-36-2
Photodegradation Half-life <sup>2</sup>	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data
Biodegradation	<b>8.6% in 28 days (measured) Not Readily biodegradable</b>	No data 8.6% in 28 days Not Readily biodegradable (RA)	No data 8.6% in 28 days Not Readily biodegradable (RA)	<b>9.1% in 28 days<sup>3</sup> (measured) Not Readily biodegradable</b>	<b>8.0% in 28 days<sup>4</sup> (measured) Not Readily biodegradable</b>	<b>8.6% in 28 days (measured) Not Readily biodegradable</b>	No data 1.5% in 28 days Not Readily biodegradable (RA)	<b>1.5% in 28 days<sup>5</sup> (measured) Not Readily biodegradable</b>	No data 8.6% in 28 days Not Readily biodegradable (RA)	No data 1.5% in 28 days Not Readily biodegradable (RA)	No data 1.5% in 28 days Not Readily biodegradable (RA)	No data 1.5% in 28 days Not Readily biodegradable (RA)
Hydrolysis Half-life	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant	Not significant
Log K <sub>oc</sub> <sup>2</sup>	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data
BCF <sup>6</sup>	71 (estimated)	3 (estimated)	3 (estimated)	71 (estimated)	71 (estimated)	3 (estimated)	6 (estimated)	3 (estimated)	71 (estimated)	3 (estimated)	3 (estimated)	71 (estimated)
Fugacity (Level III Model) <sup>2</sup>	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data	No Data
Persistence <sup>7</sup>	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)	P2 (moderate)
Bioaccumulation <sup>7</sup>	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)	B1 (low)

<sup>1</sup>American Chemistry Council; Petroleum Additives Panel; Health, Environmental, and Regulatory Task Group. 2005. Revised Robust Summary and Test Plan for Alkaryl Sulfonate Category. <http://www.epa.gov/chemrtk/pubs/summaries/alklsulf/c13206tc.htm>.

<sup>2</sup> Estimates of photodegradation, log K<sub>oc</sub>, and distribution in the environment (fugacity) do not provide meaningful information for these complex mixtures.

<sup>3</sup>Supporting chemical data, C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative (no CAS No.).

<sup>4</sup>Supporting chemical data, C<sub>20</sub>-C<sub>24</sub> alkaryl calcium salt derivative (no CAS No.).

<sup>5</sup>Supporting chemical data, magnesium long chain alkaryl sulfonate.

<sup>6</sup>USEPA. 2008. Estimation Programs Interface Suite™ for Microsoft® Windows, v3.20. United States Environmental Protection Agency, Washington, DC, USA. <http://www.epa.gov/opptintr/exposure/pubs/episuite.htm>.

<sup>7</sup>Federal Register. 1999. Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. Federal Register 64, Number 213 (November 4, 1999) pp. 60194-60204.

## 2. Environmental Effects – Aquatic Toxicity

A summary of aquatic toxicity data submitted for SIDS endpoints is provided in Table 2. The table also indicates where data for tested category members are read-across (RA) to untested members of the category.

### *Acute Toxicity to Fish*

#### ***Sulfonic acids, petroleum, calcium salts (CAS No. 61789-86-4)***

(1) Sheepshead minnow (*Cyprinodon variegatus*) were exposed to the test substance as a water accommodated fraction (WAF) under static conditions for 96 hours. The loading rates were 0 and 10,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 10,000 mg/L WAF. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, calcium salts, no effects are expected at saturation.

**No effects at saturation**

(2) Rainbow trout (*Oncorhynchus mykiss*) were exposed to the test substance as a water accommodated fraction (WAF) under static conditions for 96 hours under static-renewal conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 100 mg/L WAF. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, calcium salts, no effects are expected at saturation.

**No effects at saturation**

#### ***Sulfonic acids, petroleum, barium salts (CAS No. 61790-48-5)***

Rainbow trout (*O. mykiss*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 100 mg/L WAF. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, barium salts, no effects are expected at saturation.

**No effects at saturation**

#### ***Sulfonic acids, petroleum, sodium salts (CAS No. 68608-26-4)***

Rainbow trout (*O. mykiss*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static-renewal conditions. The loading rates were 0 and 100 mg/L and no effects were noted at the 100 mg/L WAF. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, sodium salts, no effects are expected at saturation.

**No effects at saturation**

#### ***Benzenesulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub> alkyl derivatives, calcium salts (no CAS No., supporting chemical)***

Sheepshead minnow (*C. variegatus*) were exposed to the test substance as a water accommodated fraction (WAFs) for 96 hours under static conditions. The loading rates were 0 and 10,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 100 mg/L WAF. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub> alkyl derivatives, calcium salts, no effects are expected at saturation.

**No effects at saturation**

#### ***Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased (CAS No. 71486-79-8)***

Fathead minnow (*P. promelas*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static-renewal conditions. The loading rates were 0, 100, 300 and 1,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the any of the WAF loading rates. EPA does not



consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased, no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

(1) Fathead minnow (*P. promelas*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static-renewal conditions. The loading rates were 0, 100, 300 and 1,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the any of the WAF loading rates. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts, no effects are expected at saturation.

**No effects at saturation**

(2) Sheepshead minnow (*C. variegatus*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static-renewal conditions. The loading rates were 0 and 10,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 10,000 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts, no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts (CAS No. 115733-09-0)***

Rainbow trout (*O. mykiss*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static-renewal conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 100 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts, no effects are expected at saturation.

**No effects at saturation.**

***Acute Toxicity to Aquatic Invertebrates***

***Sulfonic acids, petroleum, calcium salts (CAS No. 61789-86-4)***

*D. magna* were exposed to the test substance as a water accommodated fraction (WAF) for 48 hours under static conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 100 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, calcium salts no effects are expected at saturation.

**No effects at saturation**

***Sulfonic acids, petroleum, sodium salts (CAS No. 68608-26-4)***

*D. magna* were exposed to the test substance as a water accommodated fraction (WAF) for 48 hours under static conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 100 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, sodium salts no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased (CAS No. 71486-79-8)***

*D. magna* were exposed to the test substance as a water accommodated fraction (WAF) for 48 hours under static conditions. The loading rates were 0,100, 300 and 1,000 mg/L and no analytical measurements were made on the

WAF. No effects were noted at the 1,000 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased, no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

*D. magna* were exposed to the test substance as a water accommodated fraction (WAF) for 48 hours under static conditions. The loading rates were 0,100, 300 and 1,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 1,000 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts, no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts (CAS No. 115733-09-0)***

*Daphnia magna* were exposed to the test substance as a water accommodated fraction (WAF) for 48 hours under static conditions. The loading rates were 0,100, 300 and 1,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 1,000 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts, no effects are expected at saturation.

**No effects at saturation**

***Toxicity to Aquatic Plants***

***Sulfonic acids, petroleum, calcium salts (CAS No. 61789-86-4)***

Green algae (*S. subspicatus*) were exposed to the test substance as a water accommodated fraction (WAF) for 72 hours under static conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at any of the WAF loading rates. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, calcium salts, no effects are expected at saturation.

**No effects at saturation**

***Sulfonic acids, petroleum, sodium salts (CAS No. 68608-26-4)***

Green algae (*Scenedesmus subspicatus*) were exposed to the test substance as a water accommodated fraction (WAF) for 72 hours under static conditions. The loading rates were 0 and 100 mg/L and no analytical measurements were made on the WAF. No effects were noted at any of the WAF loading rates. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for sulfonic acids, petroleum, sodium salts, no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased (CAS No. 71486-79-8)***

Green algae (*Pseudokirchneriella subcapitata*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static conditions. The loading rates were 0, 100, 300 and 1,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at any of the WAF loading rates. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, mono-C<sub>15</sub>-C<sub>30</sub> branched alkyl and di-C<sub>11</sub>-C<sub>13</sub> branched and linear alkyl derivatives, calcium salts, overbased, no effects are expected at saturation.

**No effects at saturation**

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

Green algae (*Pseudokirchneriella subcapitata*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static conditions. The loading rates were 0, 125, 250, 500, 1,000 and 1,500 mg/L and no analytical measurements were made on the WAF. At 72 and 96 hours, biomass was reduced at the 1,500 mg/L WAF (65 and 69%, respectively). The growth rates appear not to have been affected up to 1000 mg/L WAF. Algae treated with the 1,500 mg/L WAF recovered rapidly when placed into fresh control media, indicating an algistatic effect. The 72-h and 96-h NOELs were reported as 1,000 mg/L WAF. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. The data reported suggest algistatic effects may be observed at the solubility limit when media is loaded at > 1,000 mg/L.

**Algistatic effect at saturation**

***Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts (CAS No. 115733-09-0)***

Green algae (*Pseudokirchneriella subcapitata*) were exposed to the test substance as a water accommodated fraction (WAF) for 96 hours under static conditions. The loading rates were 0, 100, 300 and 1,000 mg/L and no analytical measurements were made on the WAF. No effects were noted at the 1,000 mg/L WAF loading rate. EPA does not consider the loading rate as the no effect concentration because this concentration exceeds the solubility of the chemical. Assuming the exposure concentration in the WAF is the water solubility limit (saturation) for benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts, no effects are expected at saturation.

**No effects at saturation**

**Conclusion:** All aquatic toxicity studies submitted were conducted using Water Accommodated Fractions (WAFs) although EPA suggested that WAFs were not suitable for chemicals in this category. For all but one algae study, no acute toxicity occurred at any of the loading rates. Based on the overall weight of evidence, EPA therefore concludes that acute effects are not expected at saturation and that acute toxicity to aquatic organisms is low. However, because the dispersibility testing EPA recommended was not performed and the category members are considered water dispersible and are moderately persistent, EPA concludes chronic aquatic toxicity testing is warranted and remains a data gap.

Table 2. Summary of Environmental Effects – Aquatic Toxicity Data

Endpoints	Sulfonic acids, petroleum, calcium salts (61789-86-4)	Sulfonic acids, petroleum, barium salts (61790-48-5)	Sulfonic acids, petroleum, sodium salts (68608-26-4)	Sulfonic acids, petroleum calcium salts, overbased (68783-96-0)	Benzene sulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> alkyl derivatives, calcium salts (70024-69-0)	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives, calcium salts overbased (71486-79-8)	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives (71549-79-6)	Benzene sulfonic acid, mono and dialkyl derivatives, magnesium salts (71786-47-5)	Benzene sulfonic acid, C <sub>15</sub> -C <sub>30</sub> alkyl derivatives, sodium salts (78330-12-8)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts (115733-09-0)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased (115733-10-3)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives (115829-36-2)
Fish 96-h LC <sub>50</sub> (mg/L)	NES <sup>1</sup>	NES <sup>1</sup>	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1,2</sup>	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	No Data NES <sup>1</sup> (RA)
Aquatic Invertebrates 48-h EC <sub>50</sub> (mg/L)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	No Data NES <sup>1</sup> (RA)
Aquatic Plants 72-h EC <sub>50</sub> (mg/L)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	Algistatic at loading rate > 1,000 mg/L	No Data NES <sup>1</sup> (RA)	NES <sup>1</sup>	No Data NES <sup>1</sup> (RA)	No Data NES <sup>1</sup> (RA)

<sup>1</sup>NES = No effects at saturation (water solubility limit); <sup>2</sup>Supporting chemical data, benzenesulfonic acid, mono-C<sub>16</sub>-C<sub>24</sub>-alkyl derivatives, calcium salts

### 3. Human Health Effects

A summary of health effects data submitted for SIDS endpoints is provided in Table 3. The table also indicates where data for tested category members are read-across (RA) to untested members of the category.

#### *Acute Oral Toxicity*

The oral LD<sub>50</sub> values in rats for the members of this category range from >2.0 (CAS No. 61790-48-5) to > 16 g/kg-bw (CAS No. 71786-47-5), indicating low acute toxicity via the oral route of exposure. Individual LD<sub>50</sub> values are provided in Table 3.

#### *Acute Dermal Toxicity*

The dermal LD<sub>50</sub> values in rabbits for the members of this category range from > 2.0 (CAS Nos. 68783-96-0 and 70024-69-0) to >5.0 g/kg-bw (CAS Nos. 61789-86-4 and 115733-09-0), indicating low acute toxicity via the dermal route of exposure. Individual LD<sub>50</sub> values are provided in Table 3.

#### *Acute Inhalation Toxicity*

The inhalation LC<sub>50</sub> value in rats for one category member (CAS No. 68783-96-0) is >1.9 mg/L/4h/day (whole body exposure), indicating low acute toxicity via the inhalation route of exposure. The LC<sub>50</sub> value is provided in Table 3.

#### *Repeated-Dose Toxicity*

##### ***Sulfonic acids, petroleum, calcium salts, overbased (CAS No. 68783-96-0)***

(1) Male and female Sprague-Dawley CD rats (5/sex/dose) were administered the test substance at 0, 100, 300 and 1000 mg/kg-bw/day by dermal application for 6 hours/day, 7 days/week for 28 days followed by a 14-day recovery period for the satellite control and high-dose groups. Low incidences of erythema, desquamation and/or pinpoint scabbing were observed sporadically in the treated animals. All animals were free of edema in the study. No adverse treatment related effects on body weights, food consumption or histopathology were observed. Hematological changes [statistically significant (p not stated) increase in the mean percentage of neutrophils] were observed at 300 and 1,000 mg/kg-bw/day exposed female animals. At 1,000 mg/kg-bw/day, the females had a decrease in the mean percentage of lymphocytes on day 28. In the satellite females, a statistically significant (p not stated) decrease in the mean percentage of basophils from day 28 to 42 was within the normal range. There was a statistically significant (p not stated) decrease in the mean corpuscular hemoglobin and mean corpuscular hemoglobin concentration of the male satellite animals from day 28 to 42 (doses not specified). No other significant findings in the red blood cell parameters were observed. Two females showed increases in the mean aspartate aminotransferase and alanine aminotransferase levels at 1,000 mg/kg-bw/day. Differences from controls were all within normal ranges for the parameters tested. Observed changes in some organ weights (decrease in mean absolute brain weight of females exposed to 300 mg/kg-bw/day and mean relative decrease in adrenal and testes weights of male satellite animals) were not considered clinically relevant, as they did not correlate with any histopathological changes. Changes in satellite animals at study termination [statistically significant (p not stated) decrease in the mean relative male adrenal, brain and testes, and female adrenal and brain] were attributed to the stress from animal handling procedures during the study. Other animal handling effects included irritation at tape location and incidental liver focal necrosis in the control and exposed female rats. Irritation at the site of application was observed in all groups, including the controls; severity increasing with increasing dose.

**NOAEL = 1000 mg/kg-bw/day** (highest dose tested)

(2) Male and female Sprague-Dawley CD rats (6/sex/dose) were administered the test substance at 0, 0.0495, 0.156 and 0.260 mg/L via whole body aerosol exposure for 6 hours/day for 4 weeks followed by a 14-day post observation period. At the two higher concentrations, red nasal discharge, matted coat and decreased activity were observed. The mean body weight gain of the highest dosed males was slightly reduced over the study period. Clinical chemistry and hematological parameters indicated no treatment-related effects. Statistically significant (p not stated) incidental effects observed were increased hematocrit (low dosed females), creatinine phosphokinase (low and high dose females) and sodium (high dose females). Increases in absolute and relative lung weights were observed in the mid and high dose males and females. Except for the mid-dose female absolute lung weights, these

were statistically significant (p not stated). The accumulation of intraalveolar macrophages and hyperplasia/hypertrophy of the bronchiolar epithelium exhibited a dose-response and were considered treatment-related in the mid and high doses. At the lowest dose, the difference observed between the control and treated animals was equivocal.

**LOAEL = 0.156 mg/L** (based on increased lung weight and histopathological findings in the lungs)

**NOAEL = 0.0495 mg/L**

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

(1) Male and female Sprague-Dawley CD rats (5/sex/dose) were administered the test substance at 0, 100, 300 and 1000 mg/kg-bw/day by dermal application for 6 hours/day, 7 days/week for 28 days followed by a 14-day recovery period of the satellite control and high dose groups. One rat (300 mg/kg-bw/day female) exhibited desquamation on days 4 and 7. One rat died on day 19 (300 mg/kg-bw/day female); death was attributed to the wrapping procedure. One 1000 mg/kg-bw/day male died at study termination following blood collection. Several hematological changes, including a decrease in the mean percentage of eosinophils in low and mid dose males, were not considered treatment related as they were within normal limits for those parameters. Several hematological and clinical chemistry parameters were different from the controls in the satellite groups at the end of the recovery period. However, they were within the normal range for these parameters and were not considered treatment-related. Increase in the absolute and relative liver weights of 100 mg/kg-bw/day females and decrease in relative brain and ovary weights in the 1000 mg/kg-bw/day females at the end of the recovery period] are not considered treatment-related as they did not correlate with any histopathological findings. Livers from rats in all groups (including controls) exhibited focal or multifocal necrosis at the end of the dosing period. These changes are attributed to the animal handling procedures in dermal studies.

**NOAEL = 1000 mg/kg-bw/day** (highest dose tested)

(2) Male and female New Zealand White rabbits (15/sex/dose weighing 2 kg each) were administered the test substance at 0, 25% (~ 1,250 mg/kg-bw/day) and 100% (~ 5,000 mg/kg-bw/day) by dermal application once/day, 5 days/week for 28 days (a total of 20 applications) followed by a 4-week recovery period. One control (female) and four high-dose animals (two females and two males) died during the study. The cause of death was not established. Alopecia (loss of hair) was observed in many of the low and high dose male and female animals during the last few weeks of the study and into the recovery period. All treated animals exhibited erythema, edema, atonia, desquamation, fissuring and exfoliation, which decreased in severity into the recovery period. Less severe erythema and desquamation were also observed in the control animals. Mean body weights of the treated animals were lower than the controls. The mean total leukocyte counts, total protein and globulin of the treated animals were statistically significantly (p-value not stated) lower than the control animals at the end of the treatment period. The albumin/globulin ratios were increased. In the treated males and females, aspartate aminotransferase and glutamate pyruvate transaminase (alkaline phosphatase in females) levels increased during treatment but were unremarkable following the recovery period. In males, absolute and relative testes and epididymides weights were decreased. Absolute and relative liver weights increased in treated males and females (high dose only). Macroscopic dermal findings were consistent with in life observations. The testes of treated males appeared smaller in size than in the control animals at the end of the treatment period. Microscopic evaluations revealed treatment-related morphologic changes in the skin, testes, epididymides and the liver (high dose). Testicular changes at the high dose included aspermatogenesis, reduced number of spermatids and multifocal to diffuse tubular hypoplasia. Epithelial hypoplasia of the epididymis accompanied the testicular changes during treatment but were resolved during recovery.

**LOAEL = 25% (~ 1,250 mg/kg-bw/day)** (based on changes in body weights, changes in hematological parameters and histopathological observations)

**NOAEL = Not established**

***Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts (CAS No. 115733-09-0)***

Male and female Sprague-Dawley CD rats (5/sex/dose) were administered the test substance at 0, 50, 150, 500 and 1000 mg/kg-bw/day by oral gavage for 28 days followed by a 14-day recovery period in the control and high dose groups. Body weights of the males in the two highest dose groups were decreased during the study. Food consumption was significantly decreased (p not stated) in the 500 mg/kg-bw/day males during week 3 and in the 1000 mg/kg-bw/day females during week 2. Microscopic changes relating to irritation of the nonglandular stomach were observed in the high dose males (500 and 1000 mg/kg-bw/day) and females at doses of 150 mg/kg-bw/day and above. Edema in the submucosa was observed in the 500 mg/kg-bw/day males, as well as epithelial hyperplasia in the 1000 mg/kg-bw/day, which were resolved in the recovery period. The females exhibited edema in the

submucosa at 150 mg/kg-bw/day; edema, hemorrhaging, inflammation and ulceration at 500 mg/kg-bw/day. In the 1000 mg/kg-bw/day group, edema of the submucosa and epithelial hyperplasia were observed. The effects observed in the high-dose group were resolved during recovery.

**LOAEL = 500 mg/kg-bw/day** (based on a hemorrhaging, inflammation and ulceration in females)

**NOAEL = 150 mg/kg-bw/day**

***C<sub>20</sub>-C<sub>24</sub> Alkaryl calcium salt derivative (No CAS No., supporting chemical)***

Male and female Sprague-Dawley CD rats (6/sex/dose) were administered the test substance at 0, 100, 500 and 1000 mg/kg-bw/day by oral gavage for 29 days. No adverse treatment-related effects on body weights, food consumption, organ weights or histopathology were observed. Mean serum cholesterol levels were significantly reduced (p not stated) in the 1000 mg/kg-bw/day males and females at exposure termination and in the high dose females at study termination. Other statistically significant (p not stated) clinical and hematological parameters (not stated) were not considered treatment-related as they did not correspond with any histopathological changes.

**LOAEL = 1000 mg/kg-bw/day** (based on the reduction in mean cholesterol levels in males and females at the highest dose tested)

**NOAEL = 500 mg/kg-bw/day**

***Reproductive Toxicity***

***Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts (CAS No. 115733-09-0)***

In a one-generation reproductive toxicity study, male and female Sprague-Dawley rats (28/sex/dose) were administered the test substance at 0, 50, 167 and 500 mg/kg-bw/day via gavage once/day, 7 days/week. All F<sub>0</sub> males were dosed for 70 days prior to mating and through the completion of parturition. All females were dosed 14 days prior to mating and through day 20 of lactation. Sperm was collected from F<sub>0</sub> males for sperm count, concentration, motility and morphology evaluation. Pups were culled on lactation day 4 and 4/sex/litter were examined days 0, 4, 7, 14, and 21. The males exhibited a dose-related increase in salivation and dark material around the nose post-dosing in the mid and high dose groups. However, the mean body weight, food consumption, mating and fertility indices, absolute and relative organ weights, sperm evaluation parameters and micro/macrosopic pathologies were unremarkable. In the females, no treatment-related effects were observed in body weights, food consumption, mating and fertility indices, precoital intervals or gestation length. Two high-dose and one mid-dose female failed to deliver. No other effects were observed. No treatment-related effects were observed in the pups during lactation or during necropsy.

**NOAEL (reproductive toxicity) = 500 mg/kg-bw/day** (highest dose tested)

***Developmental Toxicity***

***Benzenesulfonic acid, C<sub>14</sub>-C<sub>24</sub> branched and linear alkyl derivatives, calcium salts (CAS No. 115733-09-0)***

In the one-generation reproductive toxicity study described previously, males exhibited a dose-related increase in salivation and dark material around the nose post-dosing in the mid- and high-dose groups. However, all reproductive parameters for both males and females were unremarkable. Two high-dose and one mid-dose female failed to deliver. No other effects were observed. No treatment-related effects were observed in the pups during lactation or during necropsy.

**NOAEL (maternal toxicity) = 500 mg/kg-bw/day** (highest dose tested)

**NOAEL (developmental toxicity) = 500 mg/kg-bw/day** (highest dose tested)

***Genetic Toxicity – Gene Mutation***

***In vitro***

***Sulfonic acids, petroleum, calcium salts, overbased (CAS No. 68783-96-0)***

In an *in vitro* in a bacterial reverse mutation assay, *Salmonella typhimurium* (TA98, TA100, TA1535, TA1537 and TA1538) were exposed to the test substance, in the presence and absence of metabolic activation and up to 5000 µg/plate. No increases in mutation frequency were reported at any concentration tested with or without metabolic activation. Positive controls gave the expected increase in the number of revertants. Beading of the test substance was observed at 5000 µg/plate in all tester strains with and without metabolic activation and at 4000 µg/plate in TA1537 (with and without metabolic activation in one replicate).

**Sulfonic acids, petroleum, calcium salts, overbased was not mutagenic in this assay.**

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

In an *in vitro* in a bacterial reverse mutation assay, *S. typhimurium* (TA98, TA100, TA1535, TA1537 and TA1538) were exposed to the test substance in the presence and absence of metabolic activation and up to 1000 µg/plate. Precipitate was observed on all plates at 1000 µg/plate with and without metabolic activation. No increases in mutation frequency were reported at any concentration tested with or without metabolic activation. Positive controls gave the expected increase in the number of revertants.

**Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts was not mutagenic in this assay.**

***Sulfonic acids, petroleum, calcium salts, overbased (CAS No. 68783-96-0)***

An *in vitro* in a mouse lymphoma (L5178Y-3.7.2C cells) mutagenicity screen was conducted using doses of 500 to 5,000 µg/mL of the test substance in the presence and absence of metabolic activation. Positive and vehicle controls elicited the appropriate responses. None of the cultures treated with test material with or without metabolic activation exhibited mutation frequencies proportionately different from solvent controls.

**Sulfonic acids, petroleum, calcium salts, overbased was not mutagenic in this assay.**

***C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative (no CAS No, supporting chemical)***

In an *in vitro* bacterial reverse mutation assay, *S. typhimurium* (TA98, TA100, TA1535, TA1537 and TA1538) were exposed to the test substance in the presence and absence of metabolic activation and up to 10,000 µg/plate. Cytotoxicity to strain TA100 was observed without metabolic activation. For the remaining strains, no increases in mutation frequency were reported at any concentration tested with or without metabolic activation. Positive controls gave the expected increase in the number of revertants.

**C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative was not mutagenic in this assay.**

***C<sub>20</sub>-C<sub>24</sub> Alkaryl calcium salt derivative (no CAS No, supporting chemical)***

In an *in vitro* in a bacterial reverse mutation assay, *S. typhimurium* (TA98, TA100, TA1535, TA1537) and *Escherichia coli* WP2uvrA were exposed to the test substance in the presence and absence of metabolic activation and up to 10,000 µg/plate. The test material formed a stable emulsion but dispersed to the top agar layer after incubation at all dose levels. Increases in revertant colonies were observed in TA1535 and WP2uvrA with metabolic activation in one of the two replicate assays. For the remaining strains, no increases in mutation frequency were reported at any concentration tested with or without metabolic activation. Positive controls gave the expected increase in the number of revertants.

**C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative was not mutagenic in this assay.**

***Genetic Toxicity – Chromosomal Aberrations***

***In vitro***

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

Chinese hamster ovary (CHO) cells were exposed *in vitro* to the test substance, with and without metabolic activation, at concentrations ranging from 10 to 160 µg/mL. The solvent and positive controls elicited the appropriate response. The test substance precipitated at doses greater than 80 µg/mL, subsequently used as the highest test dose. At 16 hours without metabolic activation, there was a statistically significant ( $p < 0.05$ ) difference between one dose level (not stated) and the control. This observation was not reproducible when the assay was repeated. There were no statistically significant ( $p < 0.05$ ) differences in the number of chromosomal aberrations at 16 hours with metabolic activation and at 40 hours with and without metabolic activation.

**Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts did not increase chromosomal aberrations in this assay.**

***Sulfonic acids, petroleum, calcium salts, overbased (CAS No. 68783-96-0)***

Chinese hamster ovary (CHO) cells were exposed to the test substance *in vitro*, with and without metabolic activation, using concentrations ranging from 10 to 160 µg/mL. The solvent and positive controls elicited the appropriate response. The test substance precipitated at doses greater than 39 µg/mL; 40 µg/mL was subsequently used as the highest test dose. In the initial 16 hr harvest, statistically significant ( $p < 0.05$ ) increases in the number of chromosomal aberrations were observed with or without metabolic activation. However, these results were not reproducible. Overall, there were no statistically significant ( $p < 0.05$ ) differences in the number of chromosomal aberrations with or without metabolic activation.

**Sulfonic acids, petroleum, calcium salts, overbased did not induce chromosomal aberrations in this assay.**



*In vivo*

***Sulfonic acids, petroleum, calcium salts, overbased (CAS No. 68783-96-0)***

A micronucleus test was conducted using Swiss albino Crl:CD-1 (ICR) BR50 mice (5/sex/dose) administered doses of test substance of 0, 500, 1000 and 2000 mg/kg via oral gavage. All vehicle, positive control and treated animals were normal after dosing and remained healthy for the study duration. There were no treatment-related increases or differences in micronuclei formation observed at any dose level. No cytotoxicity was observed. The positive control elicited the appropriate response.

**Sulfonic acids, petroleum, calcium salts, overbased did not increase micronuclei in this assay.**

***Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts (CAS No. 71786-47-5)***

A micronucleus test was conducted using CD-1 mice (5/sex/dose) administered doses of the test substance of 0, 500, 1000 and 2000 mg/kg via oral gavage. All vehicle, positive control and treated animals were normal after dosing and remained healthy for the study duration. There were no treatment-related increases or differences in micronuclei formation observed at any dose level. No cytotoxicity was observed. The positive control elicited the appropriate response. The category members are not considered to be genotoxic *in vivo* in Swiss albino mice.

**Benzenesulfonic acid, mono and dialkyl derivatives, magnesium salts did not increase micronuclei in this assay.**

***C<sub>20</sub>-C<sub>24</sub> Alkaryl calcium salt derivative (no CAS No; supporting chemical)***

A micronucleus test was conducted with Swiss albino Crl:CD-1 (ICR) BR50 mice (15 – 18/sex/dose) administered doses of the test substance of 0, 100, 200, 400 and 500 mg/kg via intraperitoneal injection. Mortality was observed at the two highest doses tested. Other clinical signs of toxicity included palpebral closure, decreased motor activity and weakness. Cytotoxicity was observed in both sexes. In males, a statistically significant (p not stated) increase in NCE/polychromatic erythrocytes (PCE) ratio was observed in the 500 mg/kg-bw/day group at 24 hours. Elevated ratios were also observed in other groups. Altered proportions of erythrocytes to nucleated cells were noted for both sexes in the treated groups. No biological or statistically significant (p not stated) increase in the number of micronucleated polychromatic erythrocytes (MPE) was observed in any treated group compared to the vehicle control. All values for individual animals were within the expected range of MPE/1000PCE expected for control animals. The variability in response observed in the treated animals was similar to that observed in the vehicle controls. The positive control elicited the appropriate response.

**C<sub>15</sub>-C<sub>21</sub> Alkaryl calcium salt derivative did not increase micronuclei in this assay.**

**Conclusion:** The acute oral toxicity for the members of this category is low. Members of the category caused irritation and point of entry effects with repeated exposures via the oral, dermal and inhalation routes. Systemic toxicity is low in the oral and dermal repeat-dose studies of rats with several category chemicals and a supporting chemical. One inhalation repeated-dose rat study of one category member showed moderate respiratory tract irritation and inflammation. A one generation study of one category member indicated low toxicity because there were no treatment-related effects on the parents or offspring for the reproductive or developmental toxicity endpoints. None of the genetic toxicity tests of the category members or supporting chemicals showed increased gene mutations or chromosomal aberrations.

Table 3. Summary of Human Health Data

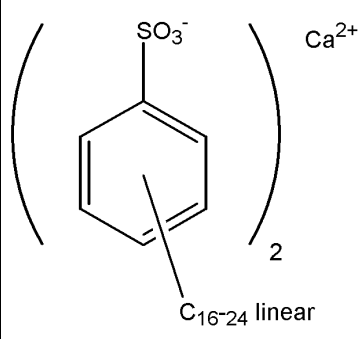
Endpoints	Sulfonic acids, petroleum, calcium salts  (61789-86-4)	Sulfonic acids, petroleum, barium salts  (61790-48-5)	Sulfonic acids, petroleum, Sodium salts,  (68608-26-4)	Sulfonic acids, petroleum calcium salts, overbased  (68783-96-0)	Benzene sulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> alkyl derivatives, calcium salts  (70024-69-0)	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives, calcium salts overbased  (71486-79-8)	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives  (71549-79-6)	Benzene sulfonic acid, mono and dialkyl derivatives, magnesium salts  (71786-47-5)	Benzene sulfonic acid, C <sub>15</sub> -C <sub>30</sub> alkyl derivatives, sodium salts  (78330-12-8)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts  (115733-09-0)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased  (115733-10-3)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives  (115829-36-2)
Acute Oral Toxicity LD <sub>50</sub> (mg/kg-bw)	> 5000	> 2000	> 5000	> 5000	> 5000 <sup>1</sup>	No Data 14,900 (RA)	14,900	>16, 000	> 5000 <sup>1</sup>	> 5000	No Data > 5000 (RA)	No Data > 5000 (RA)
Acute Dermal Toxicity LD <sub>50</sub> (mg/kg-bw)	> 5000	No Data > 5000 (RA)	No Data > 5000 (RA)	> 2000	> 2000 <sup>1</sup>	No Data > 2000 (RA)	No Data > 2000 (RA)	No Data > 2000 (RA)	No Data > 2000 (RA)	> 5000	No Data > 5000 (RA)	No Data > 5000 (RA)
Acute Inhalation Toxicity LC <sub>50</sub> (mg/L)	—*	—*	—*	> 1.9	—*	—*	—*	—*	—*	—*	—*	—*
Repeated-Dose Toxicity NOAEL/ LOAEL (mg/kg-bw/day)	No Data NOAEL between 500 and 1000 (oral) (RA)	No Data NOAEL between 500 and 1000 (oral) (RA)	No Data NOAEL between 500 and 1000 (oral) (RA)	NOAEL = 1000 (oral – highest dose)  NOAEL = 0.0495 mg/L LOAEL = 0.156 mg/L (inhalation)	NOAEL = 500 <sup>1</sup> LOAEL = 1000 <sup>1</sup> (oral)	No Data NOAEL = 1000 (dermal) NOAEL= 150 (oral) (RA)	No Data NOAEL = 1000 (dermal) NOAEL= 150 (oral) (RA)	NOAEL= 1000 (dermal – highest dose)  LOAEL = ~ 1250 (dermal, separate study, lowest dose)	No Data NOAEL = 1000 (dermal) NOAEL= 150 (oral) (RA)	NOAEL = 150 LOAEL = 500 (oral)	No Data NOAEL = 1000 (dermal) NOAEL= 150 (oral) (RA)	No Data NOAEL = 1000 (dermal) NOAEL= 150 (oral) (RA)

Table 3. Summary of Human Health Data

Endpoints	Sulfonic acids, petroleum, calcium salts  (61789-86-4)	Sulfonic acids, petroleum, barium salts  (61790-48-5)	Sulfonic acids, petroleum, Sodium salts,  (68608-26-4)	Sulfonic acids, petroleum calcium salts, overbased  (68783-96-0)	Benzene sulfonic acid, mono-C <sub>16</sub> -C <sub>24</sub> alkyl derivatives, calcium salts  (70024-69-0)	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives, calcium salts overbased  (71486-79-8)	Benzene sulfonic acid, mono-C <sub>15</sub> -C <sub>30</sub> branched alkyl and di-C <sub>11</sub> -C <sub>13</sub> branched and linear alkyl derivatives  (71549-79-6)	Benzene sulfonic acid, mono and dialkyl derivatives, magnesium salts  (71786-47-5)	Benzene sulfonic acid, C <sub>15</sub> -C <sub>30</sub> alkyl derivatives, sodium salts  (78330-12-8)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts  (115733-09-0)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives, calcium salts, overbased  (115733-10-3)	Benzene sulfonic acid, C <sub>14</sub> -C <sub>24</sub> branched and linear alkyl derivatives  (115829-36-2)
<b>Reproductive Toxicity</b> NOAEL/LOAEL (mg/kg-bw/day)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)	<b>NOAEL = 500 (highest dose)</b>	No Data NOAEL = 500 (RA)	No Data NOAEL = 500 (RA)
<b>Developmental Toxicity</b> NOAEL/LOAEL (mg/kg-bw/day)	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	<b>NOAEL = 500 (highest dose)</b>	No Data NOAEL = 500
<b>Maternal Toxicity</b>	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	No Data NOAEL = 500	<b>NOAEL = 500 (highest dose)</b>	No Data NOAEL = 500
<b>Developmental Toxicity</b>	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	NOAEL = 500 (RA)	<b>NOAEL = 500 (highest dose)</b>	NOAEL = 500 (RA)
<b>Genetic Toxicity – Gene Mutation</b> <i>In vitro</i>	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	<b>Negative</b>	<b>Negative<sup>1</sup></b>	No Data Negative (RA)	No Data Negative (RA)	<b>Negative</b>	<b>Negative<sup>2</sup></b>	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)
<b>Genetic Toxicity – Chromosomal Aberrations</b> <i>In vitro</i>	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	<b>Negative</b>	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	<b>Negative</b>	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)
<b>Genetic Toxicity – Other Effects:</b> Mouse Micronucleus ( <i>in vivo</i> )	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	<b>Negative</b>	<b>Negative</b>	No Data Negative (RA)	No Data Negative (RA)	<b>Negative</b>	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)	No Data Negative (RA)

Measured data in bold text; (RA) = Read Across; — indicates endpoint not addressed for this chemical; \* indicates endpoint is not part of the SIDS; <sup>1</sup>Supporting chemical, C<sub>20</sub>-C<sub>24</sub> alkaryl calcium salt derivative; <sup>2</sup>Supporting chemical, C<sub>15</sub>-C<sub>21</sub> alkaryl calcium salt derivative

APPENDIX

Sponsored Chemical		
Chemical Name	CAS No.	Structure <sup>1</sup>
Sulfonic Acids, Petroleum, Calcium Salts	61789-86-4	$\left( \begin{array}{c} \text{Alkyl aromatic} \\ \text{MW} = 300\text{-}400 \end{array} \text{---} \text{SO}_3^- \right)_2 \text{Ca}^{2+}$
Sulfonic Acids, Petroleum, Barium Salts	61790-48-5	$\left( \begin{array}{c} \text{Alkyl aromatic} \\ \text{MW} = 350\text{-}450 \end{array} \text{---} \text{SO}_3^- \right)_2 \text{Ba}^{2+}$
Sulfonic Acids, Petroleum, Sodium Salts	68608-26-4	$\text{Alkyl aromatic MW} = 300\text{-}400 \text{---} \text{SO}_3^- \text{Na}^+$
Sulfonic Acids, Petroleum, Calcium Salts, Overbased	68783-96-0	$\left[ \left( \begin{array}{c} \text{Alkyl aromatic} \\ \text{MW} = 350\text{-}450 \end{array} \text{---} \text{SO}_3^- \right)_2 \text{Ca}^{2+} \right]_y \cdot \left( \text{CaCO}_3 \right)_x$
Benzenesulfonic Acid, Mono-C <sub>16</sub> -C <sub>24</sub> Alkyl Derivatives, Calcium Salts	70024-69-0	

Sponsored Chemical		
Chemical Name	CAS No.	Structure <sup>1</sup>
Benzenesulfonic Acid, Mono-C <sub>15</sub> -C <sub>30</sub> Branched Alkyl and Di-C <sub>11</sub> -C <sub>13</sub> Branched and Linear Alkyl Derivatives, Calcium Salts, Overbased	71486-79-8	<p>C<sub>15-30</sub> branched</p> <p>C<sub>11-13</sub> branched and linear</p>
Benzenesulfonic Acid, Mono-C <sub>15</sub> -C <sub>30</sub> Branched Alkyl and Di-C <sub>11</sub> -C <sub>13</sub> Branched and Linear Alkyl Derivatives	71549-79-6	<p>C<sub>15-30</sub> branched</p> <p>C<sub>11-13</sub> branched and linear</p>
Benzenesulfonic Acid, Mono- and Dialkyl Derivatives, Magnesium Salts	71786-47-5	<p>R</p> <p>R' R</p>

Sponsored Chemical		
Chemical Name	CAS No.	Structure <sup>1</sup>
Benzenesulfonic Acid, C <sub>15</sub> -C <sub>30</sub> Alkyl Derivatives, Sodium Salts	78330-12-8	
Benzenesulfonic Acid, C <sub>14</sub> -C <sub>24</sub> Branched and Linear Alkyl Derivatives, Calcium Salts	115733-09-0	
Benzenesulfonic Acid, C <sub>14</sub> -C <sub>24</sub> Branched and Linear Alkyl Derivatives, Calcium Salts, Overbased	115733-10-3	
Benzenesulfonic Acid, C <sub>14</sub> -C <sub>24</sub> Branched and Linear Alkyl Derivatives	115829-36-2	

<sup>1</sup>On average, x = 10-25, y = 5-15, and R = C<sub>16</sub>-C<sub>24</sub>

## Screening Level Exposure Characterization for HPV Challenge Chemical

### Alkaryl Sulfonate Category

CAS #

61789-86-4; 61790-48-5; 68608-26-4;  
68783-96-0; 70024-69-0; 71486-79-8;  
71549-79-6; 71786-47-5; 78330-12-8;  
115733-09-0; 115733-10-3; 115829-36-2;

August 2008

Prepared by

Exposure Assessment Branch  
Chemical Engineering Branch  
Economics, Exposure and Technology Division  
Office of Pollution Prevention and Toxics  
Environmental Protection Agency  
1200 Pennsylvania Avenue, NW  
Washington, DC 20460-0001

## Screening Level Exposure Characterization Alkaryl Sulfonate Category

### Non-CBI Executive Summary

The alkaryl sulfonate category chemicals have an aggregated production and/or import volume in the range of 36 million to 211 million pounds.<sup>13</sup> The aggregated production volume includes 11 of the 12 chemicals in the category and excludes benzenesulfonic acid, mono-C16-24-alkyl derives, calcium salt (CAS# 70024-69-0), which does not have Inventory Update Reporting (IUR) submissions. Non-confidential IUR information for many of the chemicals in the alkaryl sulfonate category indicates that these chemicals are used as lubricants in the manufacturing and preparation of other chemical products. Nine of the 12 chemicals in this category have IUR submissions that indicate uses in commercial settings or consumer uses. The non-confidential IUR data are summarized later in this report.

According to the High Production Volume (HPV) Program submission,<sup>14</sup> alkaryl sulfonates are used as petroleum additives in petroleum base stocks. Petroleum additive alkaryl sulfonates are used to formulate finished lubricating oils including all types of automotive and diesel engine crankcase oils, air and water-cooled two-cycle engine oils, industrial oils, hydraulic fluids, gear oils and metal working lubricating oils. They are used as high temperature detergents to reduce deposits on pistons, engine crankcases, and hydraulic equipment parts and as rust inhibitors during industrial oil use.

*Potential Exposures to the General Population and the Environment:* There is potential for environmental releases to various media including air, water and land based on the use information from the IUR and HPV submissions and past EPA experience. Based on the totality of the information considered, especially IUR information indicating most of these chemicals are not site-limited, EPA identifies, for purposes of risk-based prioritization, a medium potential for exposure to the general population and the environment.

Persistence and bioaccumulation ratings for this chemical are P2 and B1. These ratings suggest that this chemical is moderately persistent in the environment and is not bioaccumulative.

*Potential Exposures to Workers:* Based on the totality of the information considered (including IUR data and information from the HPV submission) and in combination with Agency's professional judgment, EPA identifies, for the purposes of risk-based prioritization, a high relative ranking for the potential worker exposure. This relative ranking is based on uses that may result significant inhalation exposure and widespread dermal exposures. These uses include

---

<sup>13</sup> USEPA, 2006 Partial Updating of TSCA Chemical Inventory

<sup>14</sup> ACCPAP, 2005. High Production Volume (HPV) Challenge Program Final Submission For Petroleum Additive AlkarylSulfonate Category. Prepared by The American Chemistry Council petroleum Additives Panel Health, Environmental, and Regulatory Task Group. October 2005. Accessed 6/9/08 at <http://www.epa.gov/chemrtk/pubs/summaries/alklsulf/c13206rt.pdf>.



use in engine oils, metal working, and applications claimed to be confidential under IUR. Alkaryl sulfonate chemicals do not have OSHA Permissible Exposure Limits (PELs)<sup>15</sup>.

*Potential Exposures to Consumers:* EPA identifies, for the purposes of risk-based prioritization, a high potential for exposures to consumers from products containing these chemicals. Nine of the twelve chemicals have IUR submissions that indicate uses in commercial settings or consumer uses. Based on non-confidential IUR data, the commercial and consumer uses are lubricants, greases and fuel additives.

*Potential Exposures to Children:* EPA identifies, for the purpose of risk-based prioritization, a medium potential for exposures to children. No uses in products intended for children were reported in the IUR, nor were any found in other data sources. Exposures to children, however, may be expected to occur through the household use of some consumer products.

Below are summaries of available non-confidential information in the IUR for each of the individual chemicals in this category.

This exposure characterization was completed using IUR submissions that were available as of this writing. No information on these chemicals was found from public data sources beyond the EPA web site sources cited in this report.

---

<sup>15</sup> NIOSH, 1988. OSHA PEL Project Documentation. <http://www.cdc.gov/niosh/pel88/npelcas.html> Accessed, 5/22/08.

**Non Confidential IUR Data Summary: Sulfonic acids, petroleum, calcium salts (CAS# 61789-86-4)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites\*: Lockhart Chemical Company  
 / Flint, MI  
 Rhein Chemie Corporation / Trenton, NJ  
 Maximum number of exposed workers\*\*: between 100 and 999 (including those of  
 manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 100% by weight  
 Non-CBI physical forms\*: water- or solvent- wet solid, liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	No
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Sulfonic acids, petroleum, barium salts (CAS# 61790-48-5)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites\*: Lockhart Chemical Company  
 / Flint, MI  
 R.T. Vanderbilt, Corporate / Norwalk, CT  
 Maximum number of exposed workers\*\*: between 100 and 999 (including those of  
 manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 90% by weight  
 Non-CBI physical forms\*: other solid, liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	Confidential
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Sulfonic acids, petroleum, sodium salts (CAS# 68608-26-4)**

Manufacturing/Import Information

Production and import volume: 10 million to 50 million pounds  
 List of non-CBI companies/ sites\*: Chemtura Corporation / Middlebury, CT  
 Lockhart Chemical Company / Flint, MI  
 MacDermid, Inc. / Waterbury, CT  
 Penreco / Dickinson, TX  
 Penreco / Karns City, PA  
 Tomen America Inc. (Currently Toyota Tsusho America, Inc.) / Houston, TX\*  
 Maximum number of exposed workers\*\*: between 100 and 999 (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 100% by weight  
 Non-CBI physical forms\*: dry powder, pellets or large crystals, liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing as a reactant	Other Basic Organic Chemical Manufacturing	Intermediates
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Corrosion inhibitors and anti-scaling agents
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Processing--incorporation into formulation, mixture, or reaction product	Textile and Fabric Finishing Mills	Coloring agents, dyes
Use--nonincorporative activities	Support Activities for Printing	Other
Additional line item(s) may be claimed as CBI		

<b>Table 2                      Commercial/ Consumer Uses                      Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category                      Description</b>	<b>Highest maximum                      concentration range</b>	<b>Use in Children's Products</b>
Fabrics, textiles and apparel	Not readily available	No
Lubricants, greases and fuel additives	1% - 30%	No
Other	Less than 1%	No
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Sulfonic acids, petroleum, calcium salts, overbased (CAS# 68783-96-0)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites\*: Lockhart Chemical Company / Flint, MI  
 Idemitsu Lubricants America (Apollo America Corporation) / Jeffersonville, IN  
 Maximum number of exposed workers\*\*: 1,000 or greater (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 60% by weight  
 Non-CBI physical forms\*: liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	No
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Benzenesulfonic acid, mono-C15-30-branched alkyl and di-C (CAS# 71486-79-8)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites\*: Lockhart Chemical Company  
 / Flint, MI  
 R.T. Vanderbilt, Corporate / Norwalk, CT  
 Maximum number of exposed workers\*\*: between 100 and 999 (including those of  
 manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 90% by weight  
 Non-CBI physical forms\*: other solid, liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	Confidential
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Benzenesulfonic acid, mono-C15-30-branched alkyl and di-C (CAS# 71549-79-6)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites\*: Lockhart Chemical Company  
 / Flint, MI  
 R.T. Vanderbilt, Corporate / Norwalk, CT  
 Maximum number of exposed workers\*\*: between 100 and 999 (including those of  
 manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 90% by weight  
 Non-CBI physical forms\*: other solid, liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	Confidential
Additional line item(s) may be claimed as CBI	Confidential	Confidential



**Non Confidential IUR Data Summary: Benzenesulfonic acid, mono- and dialkyl derives, magnesium (CAS# 71786-47-5)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites: Confidential  
 Maximum number of exposed workers\*\*:  
 less than 100 (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration: Confidential  
 Non-CBI physical forms\*: liquid

\* There may be other physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1                      Industrial Processing and Use Information                      Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2                      Commercial/ Consumer Uses                      Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	No
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Benzenesulfonic acid, mono- and di-C15-30-alkyl derivs (CAS# 78330-12-8)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites\*: Arrmaz Custom Chemicals / Mulberry, FL  
 Maximum number of exposed workers\*\*: between 100 and 999 (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 100% by weight  
 Non-CBI physical forms\*: liquid

\* There may be other companies/ sites, concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Processing--incorporation into formulation, mixture, or reaction product	All Other Chemical Product and Preparation Manufacturing	Lubricants
Additional line item(s) may be claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Lubricants, greases and fuel additives	1% - 30%	No
Additional line item(s) may be claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Benzenesulfonic acid, C14-24-branched and linear alkyl deriv (CAS# 115733-09-0)**

Manufacturing/Import Information

Production and import volume: 1 million to 10 million pounds  
 List of non-CBI companies/ sites: Confidential  
 Maximum number of exposed workers\*\*:  
 less than 100 (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*:  
 up to 60% by weight  
 Non-CBI physical forms\*:  
 liquid

\* There may be other concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1                      Industrial Processing and Use Information                      Reported in 2006 IUR</b>		
<b>Processing                      Activity</b>	<b>Industrial                      Sector</b>	<b>Function in                      Ind. Sector</b>
Claimed as CBI		

<b>Table 2                      Commercial/ Consumer Uses                      Reported in 2006 IUR</b>		
<b>Commercial/ Consumer                      Product Category Description</b>	<b>Highest maximum concentration                      range</b>	<b>Use in Children's Products</b>
Claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Benzenesulfonic acid, C14-24-branched and linear alkyl deriv (CAS# 115733-10-3)**

Manufacturing/Import Information

Production and import volume: 10 million to 50 million pounds  
 List of non-CBI companies/ sites: Confidential  
 Maximum number of exposed workers\*\*: less than 100 (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 60% by weight  
 Non-CBI physical forms\*: liquid

\* There may be other concentrations and physical forms that are claimed confidential.  
 \*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1                      Industrial Processing and Use Information                      Reported in 2006 IUR</b>		
<b>Processing                      Activity</b>	<b>Industrial                      Sector</b>	<b>Function in                      Ind. Sector</b>
Claimed as CBI		

<b>Table 2                      Commercial/ Consumer Uses                      Reported in 2006 IUR</b>		
<b>Commercial/ Consumer                      Product Category Description</b>	<b>Highest maximum concentration                      range</b>	<b>Use in Children's Products</b>
Claimed as CBI	Confidential	Confidential

**Non Confidential IUR Data Summary: Benzenesulfonic acid, C14-24-branched and linear alkyl deriv (CAS# 115829-36-2)**

Manufacturing/Import Information

Production and import volume: 10 million to 50 million pounds  
 List of non-CBI companies/ sites: Confidential  
 Maximum number of exposed workers\*\*:  
 between 100 and 999 (including those of manufacturing, industrial processing and use)  
 Highest non-CBI maximum concentration\*: up to 90% by weight  
 Non-CBI physical forms\*: liquid

\* There may be other concentrations and physical forms that are claimed confidential.

\*\* There may be additional potentially exposed industrial workers that are not included in this estimate since not all submitters were required to report on industrial processing and use and/or there may be at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions.

<b>Table 1 Industrial Processing and Use Information Reported in 2006 IUR</b>		
<b>Processing Activity</b>	<b>Industrial Sector</b>	<b>Function in Ind. Sector</b>
Claimed as CBI		

<b>Table 2 Commercial/ Consumer Uses Reported in 2006 IUR</b>		
<b>Commercial/ Consumer Product Category Description</b>	<b>Highest maximum concentration range</b>	<b>Use in Children's Products</b>
Claimed as CBI	Confidential	Confidential