File No: STD/1488

November 2013

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

Cationic Surfactant in Laundry Detergent B

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals (Notification and Assessment) Act 1989* (Cwlth) (the Act) and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by the Department of Health, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of the Environment.

For the purposes of subsection 78(1) of the Act, this Public Report may be inspected at our NICNAS office by appointment only at Level 7, 260 Elizabeth Street, Surry Hills NSW 2010.

This Public Report is also available for viewing and downloading from the NICNAS website or available on request, free of charge, by contacting NICNAS. For requests and enquiries please contact the NICNAS Administration Coordinator at:

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Director
NICNAS

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SUMMARY

The following details will be published in the NICNAS *Chemical Gazette:*

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
STD/1488	Kao Australia Pty Ltd	Cationic Surfactant in Laundry Detergent B	Yes	≤ 15 tonne/s per annum	Component of liquid laundry detergent

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
Based on the available information, the notified chemical is recommended for hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia. The recommended hazard classification is presented in the table below.

Hazard classification	*Hazard statement*
Skin corrosion/irritation Cat 1	H314: Causes severe skin burns and eye damage
Serious eye damage/eye irritation Cat 1	H318: Causes serious eye damage
Acute oral Cat 3	H301: Toxic if swallowed

Based on the available information, the notified chemical is recommended for hazard classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004) with the following risk phrase:

R22: Harmful if swallowed
R38: Irritating to skin
R36: Irritating to eyes

The environmental hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals* (GHS) is presented below. Environmental classification under the GHS is not mandated in Australia and carries no legal status but is presented for information purposes.

Hazard classification	*Hazard statement*
Acute Category 1	H400, Very toxic to aquatic life
Chronic Category 1	H410, Very toxic to aquatic life with long lasting effects

Human health risk assessment
Under the conditions of the occupational settings described, the notified chemical is not considered to pose an unreasonable risk to the health of workers.

When used in the proposed manner, the notified chemical is not considered to pose an unreasonable risk to public health.

Environmental risk assessment
On the basis of the PEC/PNEC ratio and the assessed use pattern, the notified chemical is not considered to pose an unreasonable risk to the environment provided the import volume does not exceed 15 tonnes per year.

Recommendations

REGULATORY CONTROLS

Hazard Classification and Labelling

- The notified chemical should be classified as follows:
  - H314: Causes severe skin burns and eye damage
  - H318: Causes serious eye damage
  - H301: Toxic if swallowed

The above should be used for products/mixtures containing the notified chemical, if applicable, based on the concentration of the notified chemical present and the intended use/exposure scenario.

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical in the finished laundry products:
  - Avoid direct skin/eye contact with the product
  - Rinse off any skin/eye contamination with large quantity of water immediately

- A person conducting a business or undertaking at a workplace should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical in finished laundry products:
  - Impervious gloves
  - Protective clothing

  Guidance in selection of personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

- A copy of the (M)SDS should be easily accessible to employees.

- If products and mixtures containing the notified chemical are classified as hazardous to health in accordance with the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS)* as adopted for industrial chemicals in Australia, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation should be in operation.

Public Health

- The following measures should be taken by the notifier to minimise public exposure to the notified chemical:
  - Adequately label the products containing the notified chemical to avoid contact with skin and eyes, and keep out of the reach of children

Disposal

- The notified chemical should be disposed of to landfill.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by physical containment, collection and subsequent safe disposal.

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory

obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

Therefore, the Director of NICNAS must be notified in writing within 28 days by the notifier, other importer or manufacturer:

(1) Under Section 64(1) of the Act; if
- The concentration of the notified chemical in laundry detergents is proposed to exceed 6%;

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from a component of laundry detergent or is likely to change significantly;
- the amount of chemical being introduced has increased, or is likely to increase, significantly;
- the chemical has begun to be manufactured in Australia;
- additional information has become available to the person as to an adverse effect of the chemical on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

No additional secondary notification conditions are stipulated.

(Material) Safety Data Sheet
The (M)SDS of the product containing the notified chemical provided by the notifier was reviewed by NICNAS. The accuracy of the information on the (M)SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
Kao Australia Pty Ltd (ABN: 059 054 708 299)
1A The Crescent
Kingsgrove NSW 2208

NOTIFICATION CATEGORY
Standard: Chemical other than polymer (more than 1 tonne per year).

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: chemical name, other names, CAS number, molecular and structural formulae, molecular weight, analytical data, degree of purity, impurities, additives/adjuvants and import volume.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: all physico-chemical properties, acute dermal toxicity, acute inhalation toxicity, skin irritation, eye irritation, skin sensitisation, repeated dose toxicity, and *in vitro* and *in vivo* genotoxicity.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
None

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Cationic Surfactant in Laundry Detergent B

OTHER NAME(S)
Laundry Detergent B (product containing ≤ 6 % notified chemical)

MOLECULAR WEIGHT
< 500 Da

ANALYTICAL DATA
Reference NMR, FTIR and HPLC spectra were provided.

3. COMPOSITION

DEGREE OF PURITY
> 99%

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: Waxy white solid

Property	Value	Data Source/Justification
Melting Point/Freezing Point	> 200 °C	Analogue A data
Boiling Point	Not determined	Decomposition is expected before boiling
Density	935.5 kg/m^3 at 20 °C	Analogue data
Vapour Pressure	5.5 × 10^{-10} kPa at 25 °c	Calculated analogue data
Water Solubility	Not determined	The notified chemical is expected to disperse in water based on its surface activity. The critical micelle

		concentration was measured to be CMC = 0.735-0.847 g/L*.
Hydrolysis as a Function of pH	Not determined	The counter ion of the notified chemical contains hydrolysable functionality that is expected to slowly hydrolyse under environmental conditions (pH 4-9)
Partition Coefficient (n-octanol/water)	Not determined	Expected to partition to the interface between octanol and water based on its surfactant properties
Adsorption/Desorption	Not determined	Expected to accumulate at phase boundaries based on its surfactant properties and cationic functionality
Dissociation Constant	Not determined	The notified chemical is a salt and will be ionised under environmental conditions
Flash Point	Not determined	Expected to be high based on melting point
Flammability	Not determined	Not expected to be flammable
Autoignition Temperature	Not determined	Not expected to autoignite
Explosive Properties	Not determined	Contains no functional groups that would infer explosive properties
Oxidising Properties	Not determined	Contains no functional groups that would infer oxidising properties

* For full details of CMC test, refer to Appendix A

Reactivity
The notified chemical is expected to be stable under normal conditions of use.

Physical hazard classification
Based on the submitted physico-chemical data depicted in the above table, the notified chemical is not recommended for hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be imported into Australia as a component of formulated liquid laundry detergent products at up to 6% concentration.

MAXIMUM INTRODUCTION VOLUME OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	≤ 15	≤ 15	≤ 15	≤ 15	≤ 15

PORT OF ENTRY
Melbourne and Sydney.

IDENTITY OF MANUFACTURER/RECIPIENTS
Kao Australia Pty Ltd

TRANSPORTATION AND PACKAGING
Liquid Laundry detergents containing the notified chemical at up to 6% concentration will be imported and transported in 650 mL plastic bottles, packaged in cardboard containers. Products containing the notified chemical will be transported within Australia by road.

USE
The notified chemical is a surfactant that will be used as a component of domestic and professional laundry detergents at up to 6% concentration.

OPERATION DESCRIPTION
The notified chemical will not be manufactured or reformulated in Australia. The notified chemical will be imported as a component (up to 6%) of formulated liquid laundry detergent products for sale to the general public and commercial laundries.

End use
End users (members of the public and professional laundry workers) will manually measure (usually by use of container cap or measuring cup) the required volume of liquid laundry detergent (typically 1 cap full – 50 mL, containing the notified chemical at up to 6% concentration) before adding the liquid to a washing machine. During the laundry operations, the notified chemical will be diluted by water. When the end-users remove washed clothes from the washing machine, the notified chemical would have been rinsed off from the clothes.

Household consumers may also carry out hand washing and laundry pre-treatment using the laundry detergent containing up to 6% notified chemical.

6. HUMAN HEALTH IMPLICATIONS

6.1. Exposure Assessment

6.1.1. Occupational Exposure

CATEGORY OF WORKERS

Category of Worker	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transport and warehouse workers	2-3	24
Retail workers	8	200
Professional laundry workers	8-12	200

EXPOSURE DETAILS

Transport and storage
Transport and storage workers are expected to only be exposed to the notified chemical in the unlikely event of an accident. In this case, dermal and ocular exposure may occur; however, standard clean-up procedures would be in place to minimise worker exposure to the notified chemical.

Retail workers
Retail workers are not expected to have potential for exposure to the notified chemical (at up to 6% concentration) except in the event of an accidental package breach. In this case, dermal and ocular exposure may occur; however, exposure is expected to be minimised by the use of appropriate PPE including gloves and protective clothing during clean-up of any spills.

Professional laundry workers
Laundry workers may have the potential for dermal and ocular exposure to finished products containing up to 6% of the notified chemical. Exposure may occur during measuring and dispensing of the laundry product. It is recommended that workers wear gloves and protective clothing when handling the laundry products. In addition, eye contact should be avoided. During the laundry operations, the notified chemical in the finished products will be diluted by a substantial amount of water and finally rinsed off from the clothes at the end of the washing cycle. Therefore exposure from handling washed clothes would be negligible.

6.1.2. Public Exposure
Laundry products containing the notified chemical at up to 6% concentration will be available to the public. Dermal and accidental ocular exposure is possible when measuring and dispensing the laundry product into washing machines. Exposure is expected to be of short duration and infrequent (2-5days per week).

Since laundry products containing notified chemical will be sold to members of the public for home use, the public may have the potential for accidental dermal and ocular exposure to the notified chemical (up to 6% concentration). Exposure may occur during measuring and dispensing of the laundry products. It is recommended that the household users avoid direct skin and eye contact with the laundry product. During the laundry operations, the notified chemical will be diluted by a substantial amount of water and finally rinsed off

from the clothes at the end of the washing cycle. Trace quantities of residual chemical on the clothes may remain, however the levels are expected to be low.

In addition, household consumers carrying out hand washing and laundry pre-treatment using the detergents (containing up to 6% of the notified chemical) also have potential for dermal and accidental ocular exposure to the diluted detergent containing low levels of the notified chemical (< 0.06%). The low level dermal exposure may last for several minutes before the chemical is rinsed off. Potential dermal exposure from hand washing and from use of the laundry liquid to pre-treat laundry is estimated below:

Product type	**Frequency** (use/day)	**C** (%)	**Contact Area** (cm^2)	**Product Use Dilution**	**Film Thickness** (cm)	**Time Scale Factor**	**Daily systemic exposure** (mg/kg bw/day)
Laundry liquid – hand washing	1.43	0.06	1980	0.01	0.01	0.007	0.002
Laundry liquid – pre-treating	1.43	0.06	360	1	0.01	0.007	0.036
Total							0.038

Daily systemic exposure = frequency of use × concentration × body surface contact area × product concentration × film thickness on skin × time scaling factor × dermal absorption (%)/body weight

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on the notified chemical are summarised in the following table. For full details of the studies, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	LD50 >50 mg/kg bw < 300 mg/kg bw; toxic
Mutagenicity – bacterial reverse mutation	non mutagenic

Additional information on the expected health effects of the notified chemical is based on accepted analogues of the notified chemical. These analogues represent the same generic class of compound as the notified chemical and are expected to have similar toxicological effects. These analogues will be referred to as analogue A, B, C, D and E.

Endpoint	*Result and Assessment Conclusion*	*Test substance*
Rat, acute dermal toxicity	LD50 429mg/kg bw; toxic	Analogue C (EU Biocides, 2010)
Rat, acute dermal toxicity	LD50 4171 mg/kg bw; low toxicity	Analogue B (CIR, 2010)
Rabbit, skin irritation	corrosive	Analogue E
Rabbit, eye irritation	corrosive	Analogue E
Guinea pig, skin sensitisation –non-adjuvant test.	no evidence of sensitisation	Analogue D
Rat, repeat dose oral toxicity – 90 days.	NOAEL = 22 mg/kg bw/ day	Analogue B (SCCP, 2006)
Genotoxicity – in vitro chromosome aberration	non genotoxic	Analogue B (SCCP, 2006)
Rat, reproductive and developmental toxicity	NOAEL = 8.4 mg/kg bw/day	Analogue C (EU Biocides, 2010)

Toxicokinetics, metabolism and distribution.
No toxicokinetic studies are available for the notified chemical. The notified chemical is a surfactant and as such the cationic charge is expected to limit absorption across biological membranes. Dermal absorption of the notified chemical cannot be ruled out, though due to its polarity and molecular weight it is not expected to be readily absorbed.

Acute toxicity.
The acute oral toxicity of the notified chemical has been tested in rats. No deaths were observed at 50 mg/kg bw, however at the next step 2/3 animals died at 300 mg/kg bw. Thus the LD50 was determined to be LD_{50} >50 mg/kg bw < 300 mg/kg bw making the notified chemical toxic via the oral route.

The acute dermal LD50 of analogue C was found to be 429 mg/kg. However, it was noted that the observed lethality is secondary to local tissue damage rather than the result of systemic toxicity (EU Biocides, 2010). The acute dermal toxicity of analogue B has also been determined and is reported to be LD50 4.3ml/kg in rabbits (CIR, 2010). Based on these data as a worst case scenario, the notified chemical is expected to be toxic by contact with the skin.

Exposure by inhalation of the notified chemical is not expected due to the low estimated vapour pressure (5.5 $x10^{-10}$ kPa).

Irritation and sensitisation.
No irritation and sensitisation studies are available for the notified chemical. The notified chemical belongs to a group of chemicals of known skin and eye irritants.

A skin irritation test has been performed on a number of solutions of analogue E. At 5% and 10% concentration the test substance produced well-defined to moderate erythema and moderate oedema. At 1% test substance very slight to well-defined erythema were noted as well as slight oedema. Based on the effects, analogue E is classified as a severe skin irritant. An eye irritation test has also been performed on analogue B at 5% and 0.5%. At the highest concentration animals showed signs of redness, chemosis and discharge which were observed until days 14, 14 and 7, respectively. In the group receiving 0.5% test substance only conjunctival redness was observed and was resolved within 24 hours. Based on the effects, analogue B is also classified as a skin irritant.
Based on the information available, the notified chemical is expected to be irritating to the skin and eyes. It should also be noted that analogues A, B, C and D have been previously classified as corrosive to the skin and eyes by multiple notifiers (ECHA). However, full study reports were not available.

In a guinea pig maximisation test on analogue D, the substance was found to be non-sensitising. Due to the highly irritating nature of the test substance the challenge could only be performed at concentrations of 0.1% and below. However, there were no signs of irritation in the challenge phase in either the control or test animals at the doses tested.

Repeated Dose Toxicity.
No repeated dose toxicity studies are available for the notified chemical.

A 90 day repeated dose toxicity study on rats has been performed using analogue C (EU Biocides, 2010). Reduced food consumption, bodyweight gain and haemosiderine in the kidneys was observed at 113 mg/kg bw/day. These effects on the kidneys were noted to be dose-dependent and fully reversible by the end of the study. The NOAEL was determined to be 22 mg/kg bw/day.

Rats fed with analogue B for 28 days at 30, 100 and 300 mg/kg bw/day showed signs of local irritation and some signs of systemic toxicity. All animals survived till the end of the study. No effects were noted on weight or food consumption. Increased weights were noted in absolute and relative adrenal and spleen weights in males as well as increased serum ALT activity at 300 mg/kg bw/day. These changes were considered to be an indication of slight systemic toxicity. Changes related to local irritation were also noted in the forestomach and stomach. As such, the NOAEL was determined to be 100 mg/kg bw/ day (SCCP, 2006).

Based on the information provided, the notified chemical is expected to produce some systemic toxicity from repeated exposure. For the purposes of the risk assessment, a NOAEL of 22mg/kg bw/day will be used.

Mutagenicity/Genotoxicity.
The notified chemical was non-mutagenic either with or without metabolic activation in a bacterial reverse mutation assay. Analogue B was found to be non-mutagenic in a chromosome aberration test in Chinese hamster cells both with and without metabolic activation (SCCP, 2006).

Based on the information provided, the notified chemical is not expected to be genotoxic.

Toxicity for reproduction.

A number of reproductive and developmental toxicity studies have been performed using analogue C. The lowest relevant NOAEL (both maternal and prenatal) was 8.4 mg/kg bw/day. This is based on decreased body weight of dams and decreased body weights of foetuses and increased resorptions (EU Biocides, 2010).

As no further information is available relating to the dose range, duration of treatment and whether or not foetal effects were observed at doses lower than maternal toxicity, this value will not be used for the risk assessment.

Health hazard classification
Based on the available information, the notified chemical is recommended for hazard classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for industrial chemicals in Australia. The recommended hazard classification is presented in the following table.

Hazard classification	*Hazard statement*
Skin corrosion/irritation Cat 1	H314: Causes severe skin burns and eye damage
Serious eye damage/eye irritation Cat 1	H318: Causes serious eye damage
Acute oral Cat 3	H301: Toxic if swallowed

Based on the available information, the notified chemical is recommended for hazard classification according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004), with the following risk phrase(s):

R22: Harmful if swallowed
R38: Irritating to skin
R36: Irritating to eyes

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety
The notified chemical is toxic if swallowed. Based on data provided for the analogue chemicals, the notified chemical is also expected to be severely irritating to the skin and eyes and there is also potential for systemic toxicity following repeated exposure.

Workers may be exposed to the notified chemical at up to 6% concentration when handling laundry detergents. However, that the use of PPE such as gloves, goggles and protective clothing will reduce the potential for exposure. During end use, the notified chemical will be diluted by a substantial amount of water and finally rinsed off from the clothes being washed and therefore no further significant exposure is expected.

Based on the safe work practices and PPE to be used, the risk to the health and safety of workers from the use of the notified chemical as described is not considered to be unreasonable.

6.3.2. Public Health
Members of the public may come into contact with the notified chemical (up to 6% concentration) while using finished laundry detergent products. Incidental skin and eye exposure may occur and while it is not expected that gloves will be routinely worn, consumers will ordinarily wash off spills immediately. Accidental ingestion by children of the finished laundry products (up to 6 % notified chemical) may be possible and should be avoided. The notified chemical will be diluted by a substantial amount of water during the washing and finally rinsed off from the clothes at the end of the cycle. Household consumers carrying out hand washing and laundry pre-treatment using the laundry detergent may come into direct skin contact with the notified chemical.

The repeated dose toxicity potential was estimated by calculation of the margin of exposure (MoE) of the notified chemical, based on the use of laundry detergent (see section 6.1.2) and the NOAEL of 22 mg/kg bw/day for analogue B. A MoE value of 100 is considered acceptable for intra- and inter-species differences. Using the abovementioned NOAEL, a MoE of 511 was estimated.

A lower NOAEL for reproductive effects is indicated for Analogue C; however, as minimal information was available regarding this value, it was not used for the risk assessment. It is noted that even using this value, the MoE would still be considered acceptable.

Given the relatively low frequency of laundry tasks and the amount of the detergent used, the exposure to the public to the notified chemical is not expected to be high, and the risk to public health is not considered to be unreasonable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE

The notified chemical is not manufactured, reformulated or repackaged in Australia; therefore there will be no release to the environment from these activities. Environmental release during transport and storage may occur as a result of accidental spills (up to 1% of the total import volume). Spills are expected to be cleaned up by using an appropriate sorbent material and disposed of to landfill, or washed to sewers.

RELEASE OF CHEMICAL FROM USE

During use as a laundry detergent, approximately the entire volume of the notified chemical is expected to be released to sewers. Spills are expected to be cleaned up by using an appropriate sorbent material and disposed of to landfill, or washed to sewers. Residues of the notified chemical in the empty containers (up to 2%) are likely to be rinsed and will be added into the washing machine or sewer, or disposed of to landfill with the empty containers.

RELEASE OF CHEMICAL FROM DISPOSAL

The majority of the notified chemical is expected to be released to sewer. A small amount of the notified chemical is likely to be disposed of to landfill via domestic waste when empty containers are disposed of or when unused laundry detergents are discarded.

7.1.2. Environmental Fate

No environmental fate data was submitted for the notified chemical. The measured biodegradability for the analogue B, 48-65% over 28 days (reference in EI), indicates the notified chemical has a potential to biodegrade in the environment. Analogue B and the notified chemical are structurally similar and contain the same functional groups. Therefore, it is reasonable to predict the environment fate for the notified chemical based on the analogue data.

The majority of the notified chemical is expected to be released to sewage treatment plants (STPs) via domestic wastewater. Due to its cationic functional group and surface activity, a significant amount of the notified chemical is expected to sorb to sludge in STPs. The sludge containing notified chemical residues may be sent to landfill or applied to soils for land remediation. Notified chemical released to surface waters is expected to partition to suspended solids and organic matter, or to disperse and degrade. Consequently, the notified chemical is not expected be significantly bioavailable. The potential for the notified chemical to bioaccumulate is low based on its surfactant properties. The notified chemical is expected to ultimately degrade biotically and abiotically to form water and oxides of carbon, nitrogen and sulphur.

7.1.3. Predicted Environmental Concentration (PEC)

The calculation for the Predicted Environmental Concentration (PEC) is summarised in the table below. Based on the reported use in laundry detergents, it is assumed that 100% of the total import volume of the chemical is released to sewer on a nationwide basis over 365 days per year. It is evidenced by literature data that more than 99% of a representative chemical in this chemical category is expected to adsorb to waste water solids within 30 minutes of initial exposure (reference in EI). Therefore, the PEC for the notified chemical has been calculated assuming that 99% of the notified chemical will be removed during STP processes.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	15,000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	15,000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release:	41.1	kg/day

Water use	200	L/person/day
Population of Australia (Millions)	22.613	million
Removal within STP	99%	Mitigation
Daily effluent production:	4,523	ML
Dilution Factor - River	1	
Dilution Factor - Ocean	10	
PEC - River:	0.09	µg/L
PEC - Ocean:	0.01	µg/L

Partitioning to biosolids in STPs Australia-wide may result in an average biosolids concentration of 89.96 mg/kg (dry wt). Biosolids are applied to agricultural soils, with an assumed average rate of 10 t/ha/year. Assuming a soil bulk density of 1500 kg/m^3 and a soil-mixing zone of 10 cm, the concentration of the notified chemical may approximate 0.6 mg/kg in applied soil. This assumes that degradation of the notified chemical occurs in the soil within 1 year from application. Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated biosolids application, the concentration of notified chemical in the applied soil in 5 and 10 years may approximate 3 mg/kg and 6 mg/kg, respectively.

STP effluent re-use for irrigation occurs throughout Australia. The agricultural irrigation application rate is assumed to be 1000 L/m^2/year (10 ML/ha/year). The notified chemical in this volume is assumed to infiltrate and accumulate in the top 10 cm of soil (density 1500 kg/m^3). Using these assumptions, irrigation with a concentration of 0.09 µg/L may potentially result in a soil concentration of approximately 0.605 µg/kg. Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated irrigation, the concentration of notified chemical in the applied soil in 5 and 10 years may be approximately 3.03 µg/kg and 6.06 µg/kg, respectively.

7.2. Environmental Effects Assessment

No ecotoxicological data were submitted for the notified chemical. The results from ecotoxicological investigations for analogues A and B are summarised in the table below. Full study details of the algal study conducted on the analogue B can be found in Appendix C. Fish and daphnia toxicity endpoints for analogue A and B are available in a reliable international peer reviewed reports (US EPA, reference in EI).

The analogue chemicals and the notified chemical contain the same functional groups and belong to the same surfactants category. The slight differences in the length of alkyl chains and counter ions are not expected to significantly change their toxicity endpoints. Therefore, the endpoints presented below are likely to reflect the ecotoxicity of the notified chemical.

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	LC50 (96 h) = 6 mg/L (analogue A)	Toxic to fish
	LC50 (24 h) = 0.07 mg/L (analogue B)	Very toxic to fish
Daphnia Toxicity	EC50 (48 h) = 0.39 mg/L (analogue A)	Very toxic to aquatic invertebrate
	EC50 (48 h) = 0.01 mg/L (analogue B)	
Algal Toxicity	E_rC50 (72 h) = 0.058 (analogue B)	Very toxic to algae

The analogue chemicals and, by inference, the notified chemical are considered to be very toxic to aquatic organisms under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (United Nations, 2009). Furthermore, other measured ecotoxcity endpoints for surfactants belonging to the same category as the notified chemical also indicate that the notified chemical is very toxic to aquatic life (Madsen et al, 2001). Therefore, it is scientifically reasonable to use the analogue data for the classification of the notified chemical and it is formally classed as “Acute Category 1; Very toxic to aquatic life” under the GHS.

Based on the acute toxicity and lack of biodegradability data for the notified chemical, the chronic hazard of the notified chemical has been formally classed as “Chronic Category 1; Very toxic to aquatic life with long lasting effects” under the GHS.

7.2.1. Predicted No-Effect Concentration

The Predicted No-Effect Concentration (PNEC) for the notified chemical has been calculated and is presented in the table below. The PNEC is calculated based on the endpoint of the most sensitive species for the analogue chemical (daphnia, EC50 = 0.01 mg/L). Although the full study reports for the analogue chemicals were not provided, reliable endpoints are available from international peer reviewed assessment (reference in EI).

Furthermore, surfactants similar to the notified chemical are reported to have ecotoxicity endpoints falling into the same range (Madsen et al, 2001). Therefore, sufficient data are available to indicate that the endpoint values reported are in fact representative of the notified chemical. An assessment factor of 100 has been used as acute toxicity endpoints for three trophic levels are available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
EC50 (Invertebrates)	0.01	mg/L
Assessment Factor	100	
PNEC:	0.1	µg/L

7.3. Environmental Risk Assessment

Risk Assessment	***PEC µg/L***	***PNEC µg/L***	***Q***
Q - River:	0.09	0.1	0.909
Q - Ocean:	0.01	0.1	0.091

The Risk Quotients (Q = PEC/PNEC) for the notified chemical have been calculated to be < 1 for the river and ocean compartments. The calculated risk quotient indicates a relatively narrow safety margin as a result of the toxicity of the notified chemical. However, the notified chemical is expected to have the potential for biodegradation, thus it is unlikely to persist in surface waters or soils. The notified chemical is considered to have low potential for bioaccumulation. The notified chemical is unlikely to result in ecotoxicologically significant concentrations in the aquatic environment. Therefore, the notified chemical is not expected to pose an unreasonable risk to the aquatic environment based on its assessed use pattern. However, to ensure the notified chemical does not pose an unreasonable risk to the environment, i.e. to ensure $Q \leq 1$, the import volume of the notified chemical should not exceed 15 tonnes/year.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Surface Tension 28.4 mN/m at 25 °C

Method	Wilhelmy Pt plate technique
Remarks	The surface tension was measured in the range of 26.9-56.4 mN/m for the test concentrations range of 9.18×10^{-4} - 10.57 g/L. The critical micelle concentration (CMC) was determined to be 0.735-0.847 g/L in the test, and the surface tension at this concentration was measured to be 28.4 mN/m at 25 °C.
Test Facility	Kao (2013)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method.
Species/Strain	Rat/ Sprague-Dawley [Crl:CD(SD)]
Vehicle	Water
Remarks - Method	No significant protocol deviations

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
I	3F	300	0/3
II	3F	300	2/3
III	3F	50	0/3
IV	3F	50	0/3

LD50	> 50 mg/kg bw < 300 mg/kg bw
Signs of Toxicity	One animal treated with 300 mg/kg bw died within 24 hrs of administration of the test substance and cases of diarrhoea, soft stools, and mucous in stool were observed. These effects were still observed in some surviving animals treated with 300 mg/kg bw on the 2nd day and on day 3 cases of lacrimation, dirty nose, refusal to feed, lethargy and soft stools were observed. On day 4 a 2nd animal was found dead but no other abnormal clinical signs were observed. At 50 mg/kg bw no clinical signs were observed.
Effects in Organs	No effects were observed in the organs of any animal.
Remarks - Results	The oral LD50 value of the test substance was estimated to be > 50mg/kg bw and < 300 mg/kg bw.
CONCLUSION	The notified chemical is toxic via the oral route.
TEST FACILITY	Biotextech (2006a)

B.2. Irritation – skin

TEST SUBSTANCE	Analogue E
METHOD	Non OECD study
Species/Strain	Rabbit/New Zealand White
Number of Animals	6
Vehicle	Water
Observation Period	48 hours
Type of Dressing	Occlusive
Remarks - Method	8 administration sites were shaven on each animal and four sites were abraded with an 18G needle without injuring the dermis. 0.5 mL of the test substance (at 10%, 5%, or 1% concentration), water or cetyl trimethyl ammonium chloride (positive control) was added to a lint cloth and applied for 24 hours with occlusive dressing to either intact or abraded skin. Skin reactions were evaluated at 3, 24 and 48 hours after patch removal using the Draize method.

RESULTS

Lesion	*Mean Score**	*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	Intact skin / Abraded skin			

	10%	5%	1%	10%	5%	1%			
Erythema/Eschar	2.2	2.2	1.2	2.2	2.2	1.2	3	> 48 h	3
Oedema	1.7	1.7	0.2	1.7	1.7	0.2	3	> 48 h	3

*Calculated on the basis of the scores at 24 and 48 hours for EACH animal.

Remarks - Results: At the highest concentration of the test substance well-defined to moderate erythema and moderate oedema were noted for both abraded and non-abraded skin. At 5% concentration of the test substance there was little difference from the results at the highest concentration. At 1% test substance very slight to well-defined erythema were noted as well as slight oedema in one animal on both abraded and non-abraded skin.

CONCLUSION: The test substance is severely irritating to the skin.

TEST FACILITY: DSTC (2002a)

B.3. Irritation – eye

TEST SUBSTANCE: Analogue E (at 5% concentration)

METHOD: Non OECD study similar to TG 405 Acute Eye Irritation/Corrosion.

Species/Strain: Rabbit/New Zealand White

Number of Animals: 9

Observation Period: 21

Remarks - Method: 0.1 mL of either the test or cetyl trimethyl ammonium chloride (positive control) was instilled into the conjunctival sac of each animal. 1 group of three animals also had the treated eyes washed with 300 mL of lukewarm water for 30 seconds after instillation of the test solution. Treated sites were evaluated 1, 3, and 6 hours and 1, 2, 3, 4, and 7 days after installation. Additional observations were conducted on day 14 and 21 if effects persisted.

RESULTS

Lesion	*Mean Score*: Without Irrigation*		*With irrigation*	*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	0.5%	*5%*	*5%*			
Conjunctiva: redness	0	2.6	1.4	3	< 14 d	0
Conjunctiva: chemosis	0	1.2	0.2	2	< 14 d	0
Conjunctiva: discharge	0	1.2	0.3	2	< 7 d	0
Corneal opacity	0	0	0	0	-	0
Iridial inflammation	0	0	0	0	-	0

*Calculated on the basis of the scores at 24, 48, and 72 hours for ALL animals.

Remarks - Results: The group with irrigation showed signs of conjunctival redness (Day 4-7) chemosis (day 1-3) and discharge (Day 1-2). In the non-irrigation group receiving 5% notified chemical, redness, chemosis and discharge were observed until days 14, 14 and 7, respectively. In the non-irrigation group receiving 0.5% test substance only conjunctival redness was observed and was resolved within 24 hours.

The control substance produced severe eye irritation lasting up to 21 days in some instances.

CONCLUSION: The test substance causes severe eye irritation.

TEST FACILITY: DSTC (2002b)

B.4. Skin sensitisation

TEST SUBSTANCE	Analogue D
METHOD	Similar to OECD TG 406 Skin Sensitisation - guinea pig maximisation.
Species/Strain	Guinea pig/White Hartley Strain
PRELIMINARY STUDY	Maximum Non-irritating Concentration: intradermal: 0.03 %, 0.06% topical: 0.3 %
MAIN STUDY	
Number of Animals	Test Group: 10 Control Group: 5
INDUCTION PHASE	Induction Concentration: intradermal: 0.03%, 0.06% topical: 0.4%
Signs of Irritation	Intense erythema and swelling were observed with application of 0.1% concentration of test substance and above.
CHALLENGE PHASE	
1st challenge	topical: 0.1%, 0.05%, 0.03%
Remarks - Method	The challenge was performed at three different concentrations. There were no other significant protocol deviations.

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after: 1st challenge*	
		24 h	*48 h*
Test Group A	0.1	0	0
Test Group B	0.03	0	0
Test Group C	0.05	0	0
Control Group A	0.1	0	0
Control Group B	0.03	0	0
Control Group C	0.05	0	0

Remarks - Results	No signs of irritation were noted in the challenge phase in either the control or test animals.
CONCLUSION	There was no evidence of reactions indicative of skin sensitisation to the test substance under the conditions of the test.
TEST FACILITY	DSTC (1995)

B.5. Genotoxicity – bacteria

TEST SUBSTANCE	Notified chemical
METHOD	OECD TG 471 Bacterial Reverse Mutation Test. Pre incubation procedure
Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100, *E. coli*: WP2uvrA (pKM101)
Metabolic Activation System	Liver preparations (S9 mix) from rats treated with phenobarbital and 5,5-benzoflavone (BF)
Concentration Range in Main Test	a) With metabolic activation: 2.5 - 78.1 µg/plate b) Without metabolic activation: 0.7 - 19.5 µg/plate
Vehicle	water
Remarks - Method	A preliminary range finding study determined the boses used in the main test. Aliquots of either the test substance, positive or negative control solution

were tested in triplicate at 6 concentrations (0.7 - 19.5 µg/plate in the absence of S9 mix and 2.5 - 78.1 µg/plate in the presence of S9 mix). The negative control was water and positive controls were 9-aminoacridine, sodium azide and 4-nitroquinoline-1-oxide in the absence of S9 mix and 2-aminoanthracene in the presence of S9 mix.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	≥ 19.5	≥ 19.5	No precipitation	Negative
Test 2		≥ 19.5	No precipitation	Negative
Present				
Test 1		≥ 78.1	No precipitation	Negative
Test 2		≥ 78.1	No precipitation	Negative

Remarks - Results

No toxicologically significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains, at any dose of the test substance, either with or without metabolic activation.

All the positive control chemicals used in the test induced marked increases in the frequency of revertant colonies thus confirming the activity of the S9-mix and the sensitivity of the bacterial strains.

CONCLUSION

The notified chemical was not mutagenic to bacteria under the conditions of the test.

TEST FACILITY

Biotoxtech (2006b)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.2.1. Algal growth inhibition test

TEST SUBSTANCE	Analogue B
METHOD	OECD TG 201 Alga, Growth Inhibition Test.
Species	*Scenedesmus subspicatus*
Exposure Period	72 hours
Concentration Range	Nominal: Control, 0.0070, 0.020, 0.040, 0.10, 0.30 and 1.0 mg/L Actual: Not determined
Auxiliary Solvent	None
Water Hardness	~3 mg $CaCO_3$/L
Analytical Monitoring	Not applicable
Remarks - Method	The test substance was dispersed directly in culture medium. The test was conducted according to the test guideline above. The concentrations, homogeneity and stability of the test substance in the test preparations were not determined.

RESULTS

Biomass		*Growth*	
E_bC50	*NOE_bC*	*E_rC50*	*NOE_rC*
mg/L at 72 h	*mg/L*	*mg/L at 72 h*	*mg/L*
0.047	0.020	0.058*	0.020
(95% confidence limit, 0.041 – 0.054 mg/L)			

* 95% confidence limit was not calculated as the data generated did not fit the models available for the calculation of confidence limit.

Remarks - Results	Both the growth and biomass of *Scenedesmus subspicatus* were affected by the presence of the test substance over the 72-hours exposure time period. All validity criteria are satisfied. At the start of the study all the control and test cultures were observed to be clear colourless solutions. After exposure for 72 hours, the control, 0.0070, 0.020 and 0.040 mg/L test cultures were observed to be bright green dispersion. The 0.10 and 0.30 mg/L test cultures were observed to be extremely pale green dispersion. The 1.0 mg/L test cultures were observed to be clear colourless solutions. The 95% confidence limit was not calculated for the E_rC50 endpoint as the data generated did not fit the models available for the calculation of confidence limit.
CONCLUSION	The test substance and, by inference, the notified chemical are very toxic to algae.
TEST FACILITY	Safepharm (2002)

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