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AUSTRALIAN INDUSTRIAL CHEMICALS INTRODUCTION SCHEME (AICIS)

PUBLIC REPORT

Fatty acids, C_{12-14}, reaction products with sulfur trioxide, sodium salts

This Assessment has been compiled in accordance with the provisions of the *Industrial Chemicals Act 2019 (the IC Act) and Industrial Chemicals (General) Rules 2019 (the IC Rules) by following the Industrial Chemicals (Consequential Amendments and Transitional Provisions) Act 2019 (the Transitional Act) and Industrial Chemicals (Consequential Amendments and Transitional Provisions) Rules 2019 (the Transitional Rules)*. The legislations are Acts of the Commonwealth of Australia. The Australian Industrial Chemicals Introduction Scheme (AICIS) 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 Agriculture, Water and the Environment.

This Public Report is available for viewing and downloading from the AICIS website. For enquiries please contact AICIS at:

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Executive Director
AICIS

TABLE OF CONTENTS

SUMMARY

The following details will be published on the AICIS website:

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
STD/1713	BASF Australia Ltd	Fatty acids, C_{12-14}, reaction products with sulfur trioxide, sodium salts	Yes	≤ 700 tonnes per annum	Component of cosmetic and household cleaning products

CONCLUSIONS AND REGULATORY OBLIGATIONS

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

Hazard Classification	*Hazard Statement*
Acute toxicity (Category 4)	H302 – Harmful if swallowed
Skin irritation (Category 2)	H315 – Causes skin irritation
Eye irritation (Category 2A)	H319 – Causes serious eye irritation

The environmental hazard classification according to the *Globally Harmonised System of 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 Aquatic Toxicity (Category 2)	H401 - Toxic to aquatic life

Human Health Risk Assessment
Provided that the recommended controls are being adhered to, under the conditions of the occupational settings described, the assessed chemical is not considered to pose an unreasonable risk to the health of workers.

The risk to the public associated from the use of the assessed chemical at < 10% concentration in cosmetic and household products and with warnings on product labels for skin and eye irritation and safety directions for shampoo bar products at below 40% concentration, is not considered to be unreasonable.

Environmental Risk Assessment
On the basis of the PEC/PNEC ratio, the assessed chemical is not considered to pose an unreasonable risk to the environment.

Recommendations

REGULATORY CONTROLS

Hazard Classification and Labelling

- The assessed chemical should be classified as follows:
  - Acute toxicity (Category 4): H302 – Harmful if swallowed
  - Skin irritation (Category 2): H315 – Causes skin irritation
  - Eye irritation (Category 2A): H319 – Causes serious eye irritation

In the absence of skin and eye irritation data for end-use products, concentrations of the assessed chemical at ≥ 10% in end-use products warrant classification as skin irritant (Category 2) and eye irritant (Category 2A), according to GHS criteria.

The above should be used for products/mixtures containing the assessed chemical, if applicable, based on the concentration of the assessed chemical present.

Public Health

- The Delegate (and/or the Advisory Committee on Chemicals Scheduling) should consider the assessed chemical for listing on the Standard for the Uniform Scheduling of Medicines and Poisons (SUSMP) for its use in shampoo bars.
- Formulators should take into account the potential for the assessed chemical to cause skin and eye irritation when manufacturing consumer products containing the assessed chemical at ≥ 10% concentration.
- Products available to consumers containing the assessed chemical at or above 10% concentrations causing skin and eye effects should be labelled with warnings on potential adverse effects from exposure to the skin and eyes.

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following engineering controls to minimise occupational exposure to the assessed chemical during reformulation:
  - Enclosed, automated processes, where possible
  - Adequate ventilation

- 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 assessed chemical during reformulation.
  - Avoid contact with skin and eyes

- 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 assessed chemical during reformulation:
  - Safety glasses or goggles
  - 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 SDS should be easily accessible to employees.

- If products and mixtures containing the assessed chemical are classified as hazardous to health in accordance with the *Globally Harmonised System of 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.

Storage

- The handling and storage of the assessed chemical should be in accordance with the Safe Work Australia Code of Practice for *Managing Risks of Hazardous Chemicals in the Workplace* (SWA, 2012) or relevant State or Territory Code of Practice.

Emergency procedures

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

Disposal

- Where reuse or recycling are not appropriate, dispose of the assessed chemical in an environmentally sound manner in accordance with relevant Commonwealth, state, territory and local government legislation.

Regulatory Obligations

Specific Requirements to Provide Information
This risk assessment is based on the information available at the time of the application. The Executive Director may initiate an evaluation of the chemical based on changes in certain circumstances. Under Section 101 of the IC Act the applicant of the assessed chemical has post-assessment regulatory obligations to provide information to AICIS when any of these circumstances change. These obligations apply even when the assessed chemical is listed on the Australian Inventory of Industrial Chemicals (the Inventory).

Therefore, the Executive Director of AICIS must be assessed in writing within 20 days by the applicant or other introducers if:

- the final use concentration of the assessed chemical at or above 10% concentrations in cosmetic and household products and at or above 40% concentrations in shampoo bars;
- the function or use of the assessed chemical has changed from a component of cosmetics, personal care, and household cleaning products or is likely to change significantly;
- the amount of assessed chemical being introduced has increased, or is likely to increase, significantly;
- the assessed chemical has begun to be manufactured in Australia;
- additional information has become available to the person as to an adverse effect of the assessed chemical on human health, or the environment.

The Executive Director will then decide whether an evaluation of the introduction is required.

Safety Data Sheet
The SDS of the assessed chemical (and products containing the assessed chemical) provided by the applicant were reviewed by AICIS. The accuracy of the information on the SDS remains the responsibility of the applicant.

ASSESSMENT DETAILS

1. APPLICANT AND APPLICATION DETAILS

APPLICANT(S)
BASF Australia Ltd (ABN: 62 008 437 867)
Level 12, 28 Freshwater Place
SOUTHBANK VIC 3006

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

PROTECTED INFORMATION (SECTION 38 OF THE TRANSITIONAL ACT)
Data items and details exempt from publication include: concentration and analytical data.

VARIATION OF DATA REQUIREMENTS (SECTION 6 OF THE TRANSITIONAL RULES)
Schedule data requirement is varied for: hydrolysis as a function of pH, dissociation constant, flashpoint, flammability, explosive properties and oxidising properties.

PREVIOUS APPLICATION IN AUSTRALIA BY APPLICANT(S)
None

APPLICATION IN OTHER COUNTRIES
China (2019), EU REACH (2017)

2. IDENTITY OF CHEMICAL

MARKETING NAMES
Dehyton® SFA (contains the assessed chemical at 10-20% concentration)
Texapon® SFA (contains the assessed chemical at 40-50% concentration)

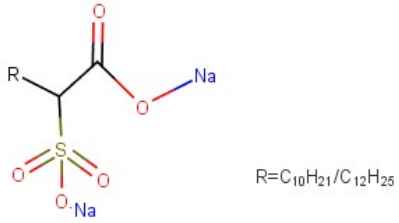
CAS NUMBER
2215087-54-8

CHEMICAL NAME
Fatty acids, C_{12-14}, reaction products with sulfur trioxide, sodium salts

OTHER NAMES
Disodium 2-Sulfolaurate
EC 942-523-5
SulfoFC C12-14, 2Na
Fatty acids, C12-14, α-sulfo, disodium salts
C12/14 Sulfo fatty acid, Na Salt

MOLECULAR FORMULA
Unspecified

STRUCTURAL FORMULA
Representative structure:



MOLECULAR WEIGHT
326 – 354 g/mol

ANALYTICAL DATA
Reference FTIR, HPLC, NMR, UV/VIS and LC/MS spectra were provided.

3. COMPOSITION

DEGREE OF PURITY
100% (UVCB)

HAZARDOUS IMPURITIES
None

NON HAZARDOUS IMPURITIES/RESIDUAL MONOMERS (> 1% BY WEIGHT)
None

ADDITIVES/ADJUVANTS
None

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: Slightly yellow solid

Property	***Value***	***Data Source/Justification***
Melting Point	Decomposes without melting at > 323 °C	Measured
Boiling Point	Decomposes without boiling at > 293 °C at 101.3 kPa	Measured
Density	1,307 kg/m^3 at 20 °C	Measured
Vapour Pressure	≤ 1.1 × 10^{-7} kPa at 20 °C	Measured
Water Solubility	63.35 g/L at 20 °C	Measured
Hydrolysis as a Function of pH	Not determined	Not determined as the assessed chemical is readily degradable
Partition Coefficient (n-octanol/water)	log Pow = -2.01 at 20 °C	Measured
Surface Tension	23.9 mN/m at 21 °C	Measured
Adsorption/Desorption	log K_{oc} = 2.43 – 3.28 at 30 °C	Measured (Chemical Safety Report, 2019)
Dissociation Constant	Not determined	The assessed chemical has two dissociation constants. It is a salt and remains dissociated.
Flash Point	Not determined	Solid
Flammability	Non-flammable	Measured
Autoignition Temperature	241 °C	Measured
Explosive Properties	Not determined	Contains no functional groups that would imply explosive properties
Oxidising Properties	Not determined	Contains no functional groups that would imply oxidising properties
Stability Testing	Stable at up to 260 °C	Measured

DISCUSSION OF PROPERTIES
For details of tests on physical and chemical properties, refer to Appendix A.

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

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

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF ASSESSED CHEMICAL (100%) OVER NEXT 5 YEARS
The assessed chemical will not be manufactured in Australia. The assessed chemical will be introduced into Australia as a solid paste or as an aqueous solution at ≤ 50% concentration for reformulation into personal care and home care products. The assessed chemical will also be introduced in finished personal care and home care products at < 10% concentration (liquid form), and in shampoo bars containing the assessed chemical at below 40% concentration.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	100	200	300	500	700

PORT OF ENTRY
Melbourne and Sydney

IDENTITY OF RECIPIENTS
BASF Australia Ltd

TRANSPORTATION AND PACKAGING
The assessed chemical will be imported for reformulation into personal care and home care products at ≤ 50% concentration by sea in 220 kg or 225 kg open head plastic drums and may also be imported in 1,000 kg intermediate bulk containers (IBCs) at a later date. Within Australia, the drums or IBCs will be transported by road to the warehouse for storage and later distribution to industrial customers by road for reformulation.

The assessed chemical will also be imported as a component of finished personal care and home care products at < 10% concentration packed in ≤ 1 L plastic bottles suitable for retail sale, and in shampoo bars containing the assessed chemical at below 40% concentration. It is also expected that the cleansing wet wipes containing the assessed chemical at < 10 % will also be imported fully finished and will be used by consumers.

USE
The assessed chemical is an anionic surfactant for use in rinse-off cosmetic (e.g. shampoos, conditioners, soap, facial cleansers, etc.) and household care products (e.g. dishwashing liquids, dishwashing tablets, hard surface cleaners, laundry liquids, wet wipes, etc.) at < 10% concentration, and in shampoo bars at below 40% concentration.

OPERATION DESCRIPTION

Reformulation
Reformulation of the assessed chemical into finished consumer goods may vary depending on the type of product and may involve both automated and manual transfer steps. Typically, reformulation processes may incorporate blending operations that are highly automated and occur in a fully enclosed/contained environment, followed by automated filling of the reformulated end-use products into containers of various sizes.

End-use
Finished personal care cosmetic products containing the assessed chemical at < 10% concentration will be used by both consumers and professionals (such as beauticians, hair dressers and childcare workers). Depending on the nature of the product, application may be by hand or through the use of an applicator.

Shampoo bars containing the assessed chemical at below 40% concentration will be used by consumers. Application will be by hand while under running water.

Homecare products containing the assessed chemical at < 10% concentration will be used by consumers and professional workers (cleaners). Dishwashing and laundry products will be used in automatic washers and for manual washing. Surface cleaning products will be applied by spray and wiped off with a cloth.

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	1-2	200-240
Formulator	8	200-240
Quality control	1-2	200-240
Packers	8	200-240
Storage	3-5	200-240
End users	8	365

EXPOSURE DETAILS

Transport and storage

Transport, storage and warehouse workers may come into contact with the assessed chemical at ≤ 50% concentration in the unlikely event of accidental rupture of containers, spills or leakages.

Reformulation

During reformulation, dermal, ocular and perhaps inhalation exposure of workers to the assessed chemical at ≤ 50% concentration may occur during weighing and transfer stages, blending, quality control analysis, and cleaning and maintenance of equipment. The applicant states that exposure is expected to be minimised through the use of mechanical ventilation and/or enclosed systems, and through the use of personal protective equipment (PPE) such as protective clothing, goggles, impervious gloves and respiratory protection, if required.

Professional end-use

Exposure to the assessed chemical in end-use products at < 10% concentration may occur in professions where the services provided involve the application of cosmetics to clients (e.g. hair dressers and workers in beauty salons), or the use of household products in the cleaning industry or the use of wet wipes in childcare facilities. The principal route of exposure will be dermal, while ocular and inhalation exposure are also possible. Workers in hair and beauty salons and childcare facilities may use some PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. If PPE is used, exposure of such workers is expected to be of a similar or lesser extent than that experienced by consumers using the products containing the assessed chemical.

6.1.2. Public Exposure

There will be widespread and repeated exposure of the public to the assessed chemical at < 10% concentration through the use of a wide range of rinse-off personal care cosmetic and homecare products, and cleansing wet wipes. When incorporated into shampoo bars, there will be widespread and repeated exposure of the public to the assessed chemical at below 40% concentration during application before it is diluted by water.

The main route of exposure will be dermal, while ocular exposure is also possible. Inhalation exposure may occur due to the formation of aerosols when applying hard surface cleaners by spray application. Inhalation exposure is unlikely from the dishwashing liquid or laundry products as the assessed chemical has low volatility and aerosols are unlikely to be formed.

Data on typical use patterns of cosmetic and household cleaning products (ACI, 2010) in which the assessed chemical will be used is shown in the following tables. In the absence of dermal absorption data, a dermal absorption (DA) of 100% was assumed for the assessed chemical (ECHA, 2017). For calculation purposes, a lifetime average female body weight (BW) of 64 kg (enHealth, 2012) was used.

Product type	Amount (mg/day)	C (%)	RF	Daily systemic exposure (mg/kg bw/day)
Shower gel	18670	10	0.01	0.292
Hand wash soap	20000	10	0.01	0.313
Shampoo	10460	10	0.01	0.163
Hair conditioner	3920	10	0.01	0.061
Facial cleanser	800	10	0.01	0.013
Shampoo bar	10460	40	0.01	0.654
Total				**1.495**

C - Concentration; RF - Retention factor; Daily systemic exposure = (Amount × C × RF × dermal absorption)/body weight

Household products (Indirect dermal exposure - from wearing clothes):

Product type	Amount (g/use)	C (%)	Product Retained (PR) (%)	Percent Transfer (PT) (%)	Daily systemic exposure (mg/kg bw/day)
Laundry liquid	230	10	0.95	10	0.341
Total					**0.341**

Daily systemic exposure = (Amount × C × PR × PT × DA)/BW; C = chemical concentration; PR = product retained; PT = product transferred; DA = dermal absorption; BW = body weight

Household products (Direct dermal exposure):

Product type	Frequency (use/day)	C (%)	Contact Area (cm^2)	Product Use C (g/cm^3)	Film Thickness (cm)	Time Scale Factor	Daily systemic exposure (mg/kg bw/day)
Laundry liquid	1.43	10	1980	0.01	0.01	0.007	0.003
Dishwashing liquid	3	10	1980	0.009	0.01	0.03	0.025
All-purpose cleaner	1	10	1980	1	0.01	0.007	0.217
Total							**0.245**

Daily systemic exposure = Frequency × C × Contact Area × Product Usage × Film Thickness × Time Scale Factor × DA/ BW; C = chemical concentration; DA = dermal absorption; BW = body weight

The worst case scenario estimation using these assumptions is for a person who is a simultaneous user of all products listed in the above tables that contain the assessed chemical at the maximum intended concentrations specified by the applicant in various product types. This would result in a combined internal dose of 2.081 mg/kg bw/day for the assessed chemical.

6.2. Human Health Effects Assessment

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

Endpoint	*Result and Assessment Conclusion*
Acute oral toxicity – rat	LD50 > 500 and < 2,000 mg/kg bw; harmful
Acute dermal toxicity – rat	LD50 > 2,000 mg/kg bw; low toxicity
Skin corrosion – *in vitro* EpiDerm™ reconstructed human epidermis test	non-corrosive
Skin irritation – *in vitro* EpiDerm™ reconstructed human epidermis test	Irritant
Eye irritation – *in vitro* bovine corneal opacity and permeability (BCOP) test	non-irritant at 10% concentration
Eye irritation – *in vitro* EpiOcular™ test	Irritant
Eye irritation – rabbit	Irritant
Skin sensitisation – guinea pig, Buehler test	no evidence of sensitisation at up to 5% concentration
Repeat dose oral toxicity – rat, 28 days	NOAEL > 1,057 mg/kg bw/day in males, 346 mg/kg bw/day in females

Endpoint	*Result and Assessment Conclusion*
Mutagenicity – bacterial reverse mutation test	non mutagenic
Genotoxicity – *in vitro* gene mutation test in Chinese hamster ovary cells (HPRT LOCUS ASSAY)	non mutagenic
Genotoxicity – *in vitro* micronucleus assay in V79 cells	non-clastogenic

Toxicokinetics
Given its relatively low molecular weight (< 600 g/mol) and high water solubility (63.3 g/mL) the assessed chemical is likely to be absorbed across the biological membrane. However, given its low partition coefficient (log Pow = -2.01 at 20 °C), limited dermal absorption is expected. As the assessed chemical is soluble in water, oral and gastrointestinal absorption is expected to be high.

Acute Toxicity
The assessed chemical was found to be harmful to rats via the oral route, with LD50 determined to be between 500 and 2,000 mg/kg bw in rats. The assessed chemical was found to be of low acute toxicity to rats via the dermal route (LD50 > 2000 mg/kg bw).

No acute inhalation toxicity data were provided on the assessed chemical. Due to the low vapour pressure of the assessed chemical, inhalation exposure is not expected.

Irritation and Sensitisation
The assessed chemical was determined as not corrosive in an *in vitro* skin corrosion test using the EpiDerm™ reconstructed human epidermis model. However, the assessed chemical was considered irritating to the skin in an *in vitro* skin irritation test using the EpiDerm™ reconstructed human epidermis model. The relative mean tissue viability for the assessed chemical was 18.4% (less than or equal to 50%) as compared to the negative control tissues; the assessed chemical was considered a skin irritant, warranting hazard classification

The assessed chemical (10% concentration) was not considered an eye irritant in an *in vitro* bovine corneal opacity and permeability (BCOP) test. However, in an *in vitro* eye irritation study using the EpiOcular™ cornea-like epithelial model, the relative viability of the test substance was 1.6%. Destruction of the tissues in these tests were attributed to the irritant effect of the test substance. Therefore, the assessed chemical was considered to be an eye irritant under the conditions of the test.

Based on *in vivo* eye irritation study conducted in rabbits (according to the OECD TG 405), the assessed chemical was irritating to the eyes of rabbits. Moderate redness and chemosis persisted in most animals at the 72 hour observation and the symptoms reduce to slight (grade 1) at the day 7 observation. The symptoms were resolved at the day 14 observation. Based on the results of this study, the assessed chemical warrants classification as a Category 2A eye irritant according to the GHS.

The assessed chemical at 5% concentration was not a skin sensitiser in a guinea pig (Buehler test).

Repeated Dose Toxicity
A repeated dose oral toxicity study on the assessed chemical was conducted in rats, in which the test substance was administered in the diet at 85.6 (M), 90 (F) (1,000 ppm), 337.3 (M), 346.2 (F) (4,000 ppm) and 1,057.1 (M), 1083.2 (F) (12,000 ppm) mg/kg bw/day for 28 consecutive days. The No Observed Adverse Effect Level (NOAEL) was established as 346 mg/kg bw/day in females, based on statistically significant and dose related occurrence of anaemia (reduction in haemoglobin and haematocrit levels) in high dose females. The NOAEL for males was > 1,057 mg/kg bw/day (the highest dose tested).

Mutagenicity/Genotoxicity
The assessed chemical tested negative in a bacterial reverse mutation assay, in an *in vitro* gene mutation test in Chinese hamster ovary cells (HPRT LOCUS ASSAY) and in an *in vitro* micronucleus assay with V79 cells.

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

Hazard Classification	*Hazard Statement*
Acute toxicity (Category 4)	H302 – Harmful if swallowed

Skin irritation (Category 2)	H315 – Causes skin irritation
Eye irritation (Category 2A)	H319 – Causes serious eye irritation

6.3. Human Health Risk Characterisation

Based on available toxicological data, the assessed chemical could be harmful via the oral route and is irritating to the skin and eyes. Given the low partition coefficient (log Pow = -2.01 at 20 °C) and ionic nature of the assessed chemical, dermal absorption is likely to be limited. Inhalation exposure is not expected to be significant due to the low vapour pressure of the assessed chemical.

6.3.1. Occupational Health and Safety

Workers may experience dermal, ocular and perhaps inhalation exposure to the assessed chemical at ≤ 50% concentration at reformulates sites during weighing and transferring the assessed chemical to the blending vessel, blending operations, quality testing, and equipment cleaning and maintenance. However, exposure to the assessed chemical is expected to be limited during reformulation with the proposed use of local ventilation, enclosed/automated processes and through the use of PPE such as protective clothing, goggles, impervious gloves and respiratory protection, if required.

During end-uses, professional workers may be exposed to the assessed chemical in end-use products at < 10% concentration in professions where the services provided involve the application of cosmetics to clients (e.g. hair dressers and workers in beauty salons). The principal route of exposure will be dermal, while ocular and inhalation exposure are also possible following spray application. While the assessed chemical will not be skin and eye irritant at this concentration (< 10%), hair dressers and workers in beauty salons may use some PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. If PPE is used, exposure of such workers is expected to be of a similar or lesser extent than that experienced by consumers using the products containing the assessed chemical.

Exposure to the assessed chemical in end-use products at < 10% concentration may occur in professions following the use of household products in the cleaning industry. The principal route of exposure will be dermal, while ocular and inhalation exposure are also possible following spray application. Workers may use some PPE to minimise repeated exposure, and good hygiene practices are expected to be in place. Furthermore, as the assessed chemical will not be skin and eye irritant at this concentration (< 10%), risk is expected be minimal.

The cleansing wet wipes containing the assessed chemical at < 10% concentration will be used directly by hand in childcare facilities. However, only a small percentage of liquid from the wet wipe is expected to be left as residual on the skin. As the assessed chemical at this concentration (< 10%) will not be a skin irritant, the risk is expected to be limited.

Therefore, provided adequate control measures are in place to minimise worker exposure, including the use of automated processes during reformulation and the use of PPE, the risk to workers from use of the assessed chemical is not considered to be unreasonable.

6.3.2. Public Health

Members of the public may experience repeated exposure to the assessed chemical through the use of rinse-off cosmetic and household products containing the assessed chemical at < 10% concentration, and the use of rinse-off personal care products in shampoo bar form containing the assessed chemical at below 40% concentration.

The assessed chemical is a skin and an eye irritant, however, irritants effects are not expected from the use of products containing the assessed chemical at the proposed (< 10%) use concentration in liquid cosmetic and household products. There is potential for irritation effects when using personal care products in shampoo bar form due to higher (< 40%) concentrations of the assessed chemical prior to dilution with water during application and before the product is rinsed off. The risk to the public would be mitigated by safe use instructions and warnings on products.

The cleansing wet wipes containing the assessed chemical will be used directly by hand, however, only a small percentage of liquid from the wet wipes containing the assessed chemical at < 10% concentration is expected to be left as residual on the skin. Irritation effects from wet wipes are not expected due to the concentration of the assessed chemical in them (< 10%).

The repeat dose toxicity potential was estimated by calculation of the margin of exposure (MoE) of the assessed chemical using the worst case exposure scenario from use of multiple products by an individual with total exposure of 2.081 mg/kg bw/day. Using a NOAEL of 346 mg/kg bw/day for the assessed chemical (derived from a 28 day repeated dose toxicity study in rats, Section 6.2), the margin of exposure (MoE) was estimated to be 166. A MoE value ≥ 100 is generally considered to be acceptable for taking into account intra- and inter-species differences, therefore, the MoE is considered to be acceptable.

Overall, the risk to the public associated from the use of the assessed chemical at < 10% concentration in cosmetic and household products and with warnings on product labels for skin and eye irritation and safety directions for shampoo bar products at below 40% concentration, 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 assessed chemical is not manufactured in Australia. Any accidental spills are to be collected and disposed of in accordance with local government regulations. Wash waters from equipment cleaning, containing the assessed chemical are expected to be collected and disposed of to landfill. Some of the assessed chemical in waste water may be released to sewer.

RELEASE OF CHEMICAL FROM USE

A majority of the assessed chemical is expected to be washed into sewer waters as a part of its use in various cosmetic and household products where it will be treated in sewage treatment plants nationwide before being released into surface waters.

RELEASE OF CHEMICAL FROM DISPOSAL

A small proportion of the assessed chemical is expected to remain as residues in empty product containers. These containers are expected to be either recycled or disposed of to domestic landfill.

7.1.2. Environmental Fate

Following its use in cosmetic products and household cleaning products, the assessed chemical is expected to be primarily released into the sewer system and treated at sewage treatment plants before release to surface waters nationwide.

The assessed chemical is readily biodegradable (73% biodegradation after 28 days). For details, refer to Appendix C. The assessed chemical is not expected to bioaccumulate due to its low log Pow (-2.01). Some of the assessed chemical may remain in the end use and bulk containers, which are either recycled or disposed of to landfill. In surface waters and landfill, the assessed chemical is expected to degrade into water, sodium salts and oxides of carbon and sulphur.

7.1.3. Predicted Environmental Concentration (PEC)

The use pattern will result in most of the assessed chemical being washed into the sewer. The predicted environmental concentration (PEC) has been calculated based on the realistic scenario with 100% release of the assessed chemical into sewer systems nationwide over 365 days per annum. The extent to which the assessed chemical is removed from the effluent in STP processes is based on the physico-chemical properties and its ready biodegradability, modelled by SimpleTreat 3.0 (Struijs, 1996) and is estimated as 67%. The PEC in sewage effluent on a nationwide basis is estimated as follows:

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	700,000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	700,000.000	kg/year
Days per year where release occurs	365	days/year
Daily chemical release:	1917.81	kg/day
Water use	200.0	L/person/day
Population of Australia (Millions)	24.386	million
Removal within STP	67%	**Mitigation**

Daily effluent production:	4,877	ML
Dilution Factor – River	1.0	
Dilution Factor – Ocean	10.0	
PEC – River:	129.76	µg/L
PEC – Ocean:	12.98	µg/L

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 assessed 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 130 µg/L may potentially result in a soil concentration of approximately 865 µg/kg. Since the assessed chemical is readily biodegradable, accumulation in soil is not expected.

7.2. Environmental Effects Assessment

The results from ecotoxicological investigations conducted on the assessed chemical are summarised in the table below. Details of these studies can be found in Appendix C. As the assessed chemical is a surfactant the ecotoxicological tests were conducted on the water accommodated fraction (WAF) and water soluble fraction (WSF) to exclude aqueous dispersions. The measured water solubility is likely to include these dispersions.

Endpoint	*Result*	*Assessment Conclusion*
Fish Acute Toxicity	LL50 = 5.72 mg/L†	Toxic to fish
	LL50 = 17.7 mg/L‡	Harmful to fish
Daphnia Acute Toxicity	EL50 = 93 mg/L	Harmful to aquatic invertebrates
Algal Acute Toxicity	EL50 = 116 mg/L	Not harmful to algal growth
Daphnia Chronic Toxicity	NOEC = 10 mg/L	Very slightly toxic to aquatic invertebrate*
Inhibition of Bacterial Respiration	EC50 > 1000 mg/L	Not harmful to bacterial respiration
Soil Microorganisms Nitrification inhibition	EC50 > 1000 mg/L	Not harmful to microbial nitrification.

* Only study summary provided (CSR 2019)
† Water accommodated fraction (WAF).
‡ Water soluble fraction

Based on the above ecotoxicological endpoints for the assessed chemical, it is expected to be acutely toxic to fish and harmful to daphnids. Therefore, under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) (United Nations, 2009), assessed chemical is formally classified as “Acute Category 2; Toxic to aquatic life”.

7.2.1. Predicted No-Effect Concentration

The Predicted No-Effect Concentration (PNEC) was calculated using the most sensitive endpoint, taking into account that two acute fish studies were conducted. The lowest value of the geometric mean of the LL50 values for fish (10.1 mg/L) and the NOEC for chronic toxicity to daphnia (10.0 mg/L) was used for calculating the PNEC. The NOEC for chronic toxicity to daphnia was found to be marginally lower and the PNEC was calculated using this value. An assessment factor of 50 is used as three measured acute endpoints and a chronic endpoint are available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
Chronic Toxicity to daphnia (NOEC)	10.0	mg/L
Assessment Factor	50	
Mitigation Factor	1.00	
PNEC	200	µg/L

The Predicted No-Effect Concentration (PNEC) was also calculated based on the terrestrial toxicity endpoint (EC50 soil microorganisms) with an assessment factor of 1000 as there is data for only one endpoint.

Predicted No-Effect Concentration (PNEC) for the Terrestrial Compartment		
Soil microorganisms EC50	1000	mg/kg
Assessment Factor	1000	
Mitigation Factor	1.00	
PNEC	1000	µg/kg

7.3. Environmental Risk Assessment

The Risk Quotient (Q = PEC/PNEC) was calculated based on the predicted PEC and PNEC.

Risk Assessment	PEC (µg/L)	PNEC (µg/L)	Q
Q – River	129.8	200	**0.65**
Q – Ocean	13.0	200	**0.065**

The Risk Quotient (Q = PEC/PNEC) for the terrestrial environment was calculated as follows.

Risk Assessment	PEC (µg/kg)	PNEC (µg/kg)	Q
Q - soil	865	1000	0.87

The assessed chemical is not persistent and is not likely to bioaccumulate. The assessed used pattern results in Q values of less than 1 for the aquatic and terrestrial environment, indicating that the assessed chemical is unlikely to reach ecotoxicologically significant concentrations. Therefore on the basis of the aquatic and the terrestrial PEC/PNEC ratios, the assessed chemical is not considered to pose an unreasonable risk to the environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point Decomposes without melting at > 323 °C

Method	EC Council Regulation No 440/2008 A.1 Melting/Freezing Temperature
Remarks	Determined using differential scanning calorimetry (capsulated crucible). No melting point was observed up to 323 °C. From 323 °C the test substance showed a thermal decomposition. The difference in decomposition temperatures in the melting and boiling results (see below) is considered by the study authors to be due to different measuring conditions (melting- capsulated crucible; boiling – partially capsulated crucible)
Test Facility	Henkel (2016a)

Boiling Point Decomposes without boiling at > 293 °C at 101.3 kPa

Method	EC Council Regulation No 440/2008 A.2 Boiling Temperature
Remarks	Determined using differential scanning calorimetry (partially capsulated crucible)
Test Facility	Henkel (2016b)

Density 1,307 kg/m^3 at 20 °C

Method	OECD TG 109 Density of Liquids and Solids EC Council Regulation No 440/2008 A.3 Relative Density
Remarks	Pycnometer method
Test Facility	Henkel (2016c)

Vapour Pressure ≤ 1.1×10^{-7} kPa at 20 °C

Method	EC Council Regulation No 440/2008 A.4 Vapour Pressure
Remarks	DSC method
Test Facility	Henkel (2016d)

Water Solubility 63.35 g/L at 20 °C

Method	OECD TG 105 Water Solubility
Remarks	Column Elution Method. Water solubility was determined by integrating the entire peak group of the assessed chemical in the obtained chromatograms and the pH of the solution was 5.94.
Test Facility	Henkel (2016i)

Partition Coefficient (n-octanol/water) log Pow = -2.01 at 20 °C

Method	In house method
Remarks	Partition coefficient derived from individual solubilities in 1-octanol and water. Individual solubilities were determined according to the principals described in OECD TG 105. Solubility in 1-octanol was determined to be 620 mg/L at 20°C
Test Facility	Henkel (2016j)

Surface Tension 23.9 mN/m at 21 °C

Method	OECD TG 115 Surface Tension of Aqueous Solutions EC Council Regulation No 440/2008 A.5 Surface Tension
Remarks	Concentration: 1g/L
Test Facility	Henkel (2016e)

Adsorption/Desorption – screening test log K_{oc} = 2.43 – 3.28 at 30 °C

Method	OECD TG 121 Adsorption – Desorption om Soil and Sewage Sludge
Remarks	HPLC method

Test Facility Henkel AG (Dr. O. Seiler, 2018)

Flammability Non-flammable

Method EC Council Regulation No 440/2008 A.10 Flammability (Solids)
Remarks In a preliminary test, a particle train of the test substance ignites and the flame ceases within 2 minutes without propagation. Under the conditions of the test the test substance is not classified as a flammable solid.
Test Facility Henkel (2016g)

Autoignition Temperature 241 °C

Method EC Council Regulation No 440/2008 A.16 Relative Self-Ignition Temperature for Solids
Test Facility Henkel (2016g)

Stability Testing Stable up to 260 ºC

Method OECD TG 113 Screening Test for Thermal Stability and Stability in Air
Remarks DSC method
Test Facility Henkel (2016h)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute Oral Toxicity – Rat

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method (2001)
Species/Strain	Rat/Wistar/Crl:WI (Han) SPF
Vehicle	Deionised water
Remarks – Method	No protocol deviations.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw)*	*Mortality*
1	3F	2,000	3/3
2	3F	500	0/3
3	3F	500	0/3

LD50	> 500 and < 2,000 mg/kg bw
Signs of Toxicity	Group 1 Impaired general state, dyspnea and piloerection were observed in all 3 animals 4-5 hours after dosing. All animals were found dead at day 1 observation. Group 2 Impaired general state and piloerection were observed in all 3 animals at 2 hour until 5 hour or day 1 observations. Group 3 All animals showed impaired general state and piloerection at 3 hour until 5 hour observations, and one of these animals also showed dyspnea.
Effects in Organs	Congested kidneys, filled stomach with mustard coloured contents and discoloured (red) glandular stomach and small intestine were observed in group 1 animals at necropsy. No abnormalities were observed in groups 2 and 3 animals at necropsy.
Remarks – Results	Normal bodyweight gain was observed in all surviving (groups 2 and 3) animals during the study.
CONCLUSION	The assessed chemical is harmful via the oral route.
TEST FACILITY	Bioassay (2017a)

B.2. Acute Dermal Toxicity – Rat

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 402 Acute Dermal Toxicity (1987)
Species/Strain	Rat/Wistar / Crl:WI (Han) SPF
Vehicle	Deionised water
Type of dressing	Semi-occlusive
Remarks – Method	No protocol deviations.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw)*	*Mortality*
1	5M/5F	2,000	0/10

LD50	> 2,000 mg/kg bw
Signs of Toxicity – Local	

	Test item-related local effects recorded during the course of the study included: very slight to well-defined erythema (grade 1 to 2), very slight oedema (grade 1), incrustations, scaling, eczema like skin lesions and weeping areas of the skin.
Signs of Toxicity – Systemic	No signs of systemic toxicity observed during the study.
Effects in Organs	No abnormalities were noted during necropsy.
Remarks – Results	Normal bodyweight gain was observed in all male animals during the study. In the first week, a slight loss of bodyweight was observed in three females, while the other two females showed a stagnation of bodyweight gain. In the second week two females showed a normal bodyweight gain, while the other three animals showed a stagnation of bodyweight gain. As slight loss of body weight or stagnation of body weight is commonly known for females after dermal applications, this stagnation is considered to be unspecific.
CONCLUSION	The assessed chemical is of low acute toxicity via the dermal route.
TEST FACILITY	Bioassay (2017b)

B.3. Skin Corrosion – *In Vitro* Reconstructed Human Epidermis Test

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 431 *In vitro* Skin Corrosion – Reconstructed Human Epidermis (RHE) Test Method (2016) EC Council Regulation No 440/2008 B.40 bis. *In vitro* Skin Corrosion – Human Skin Model Test
Vehicle	Water
Remarks – Method	GLP Certificate\ EpiDerm™ model No significant protocol deviations. Positive and negative controls were run in parallel with the test substance. Negative control: deionised water Positive control: 8N potassium hydroxide solution The MTT [(3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide, thiazolyl blue] assay was used to determine cell viability.

RESULTS

Exposure 3 minutes

Test Material	*Mean OD_{570} of Duplicate Tissues*	*Relative Mean Viability (%)**	*SD of Relative Mean Viability*
Negative control	1.755	100	2.2
Test substance	1.718	97.9	1.1
Positive control	0.313	17.8	4.8

OD = optical density; SD = standard deviation; *Relative to the negative control, which is assigned a value of 100%.

Exposure 1 hour

Test Material	*Mean OD_{570} of Duplicate Tissues*	*Relative Mean Viability (%)**	*SD of Relative Mean Viability*
Negative control	1.926	100	3.3
Test substance	1.416	73.5	21.6
Positive control	0.137	7.1	7.0

OD = optical density; SD = standard deviation; *Relative to the negative control, which is assigned a value of 100%.

Remarks – Results	The test substance was shown not to directly reduce MTT. The relative mean tissue viability for the test substance as compared to the negative control was 97.9% (3 minutes exposure) and 73.5% (1 hour exposure). Given that the relative mean tissue viability for the test substance was > 50%, after 3 minute exposure and > 20% after 1 h exposure, the test substance is not classified as a skin corrosive according to the test guidelines, using GHS criteria. The positive and negative controls gave satisfactory results, confirming the validity of the test.
CONCLUSION	The assessed chemical was considered non-corrosive to the skin under the conditions of the test.
TEST FACILITY	BASF (2016a)

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B.4. Skin Irritation – *In Vitro* Reconstructed Human Epidermis Test

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 439 *In vitro* Skin Irritation: Reconstructed Human Epidermis Test Method (2015) EC Council Regulation No 440/2008 B.40 bis. *In vitro* Skin Corrosion – Human Skin Model Test
Vehicle	Water
Remarks – Method	GLP Certificate\ EpiDerm™ model No significant protocol deviations. Positive and negative controls were run in parallel with the test substance: Negative control: phosphate buffered saline Positive control: 5% sodium dodecyl sulfate in waterNo space hereThe MTT [(3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide, thiazolyl blue] assay was used to determine cell viability.

RESULTS

Test Material	*Mean OD_{570} of Triplicate Tissues*	*Relative Mean Viability (%)**	*SD of Relative Mean Viability*
Negative control	2.154	100	8.0
Test substance	0.397	18.4	4.9
Positive control	0.072	3.3	0.2

OD = optical density; SD = standard deviation
*Relative to the negative control, which is assigned a value of 100%.

Remarks – Results	A chemical is considered as irritant if the mean relative tissue viability with a test material is less than or equal to 50%, as compared to the negative control tissues concurrently treated with sterile PBS. As the relative mean tissue viability for the test substance as compared to the negative control was 18.4%, the assessed chemical showed skin irritation potentials. The positive and negative controls gave satisfactory results, confirming the validity of the test.
CONCLUSION	The assessed chemical was considered irritating to the skin under the conditions of the test.
TEST FACILITY	BASF (2016a)

B.5. Eye Irritation – *In Vitro* Bovine Corneal Opacity Test (BCOP)

TEST SUBSTANCE	Assessed chemical (10% Concentration)
METHOD	OECD TG 437 Bovine Corneal Opacity and Permeability Test Method for Identifying Ocular Corrosives and Severe Irritants (July 2013)
Vehicle	None
Remarks – Method	Two positive controls were used: ethanol (100%) (PC1) and dimethylformamide (100%) (PC2). No significant protocol deviations. Negative control: deionised water The surfactant-based test substance was assessed by a single application of 750 µL of a 10% diluted test-substance preparation in water to the epithelial surface of isolated bovine corneas. Corneal opacity and permeability were measured and were used to calculate an *In Vitro* Irritancy Score (IVIS) of the test substance.

RESULTS

Test Material	*Mean Opacities of Triplicate Tissues (SD)*	*Mean Permeabilities of Triplicate Tissues (SD)*	*IVIS (SD)*
Negative control	6.6 (2.3)	0.004 (0.002)	6.6 (2.3)
*Test substance (10%)**	1.1 (1.9)	0.085 (0.058)	2.4 (1.2)
*Positive control (PC1)**	23.8 (1.7)	0.695 (0.171)	34.3 (2.2)
*Positive control (PC2)**	88.6 (3.6)	0.544 (0.125)	96.8 (2.5)

SD = Standard deviation; IVIS = in vitro irritancy score
*Corrected for background values

Remarks – Results	The negative control gave IVIS of 6.6 (which is above 3) but this IVIS was within the mean values of the negative historical control data with two standard deviation. No adverse irritation findings were observed for negative control at the histopathological evaluation. The IVIS of the test substance was 2.4. An IVIS ≤ 4.5 is considered as borderline in predicting no classification for eye irritation according to the test guideline. The positive controls gave satisfactory results confirming the validity of the test system.
CONCLUSION	The test substance (assessed chemical at 10% concentration) was not considered an eye irritant under the conditions of the test.
TEST FACILITY	BASF (2016b)

B.6. Eye Irritation – *In Vitro* EpiOcular™ Test

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 492 Reconstructed human Cornea-like Epithelium (RhCE) test method for identifying chemicals not requiring classification and labelling for eye irritation or serious eye damage (2015)
Vehicle	Nil
Remarks – Method	Negative control: deionised water Positive control: methyl acetate (100%) No significant protocol deviations.

RESULTS

Test Material	*Mean OD_{570} of Duplicate Tissues*	*Relative Mean Viability (%)*
Negative Control	1.583	100
Test Substance	0.026	1.6
Positive Control	0.532	33.6

OD = optical density

Remarks – Results

The relative mean viability of the test substance was 1.6%. As detachment and damage of the tissues was noted during the washing procedure, a second test run was performed to clarify the result.

The mean viability of the test-substance treated tissues for the second test run was also 1.6%. Detachment of the tissues during the washing period also occurred again. Thus, the 2nd test run verified the results of the 1st test run and confirmed that the destruction of the tissues is attributed to the irritant effect of the test substance.

The controls gave satisfactory results confirming the validity of the test system.

CONCLUSION

The assessed chemical showed eye irritant potential under the conditions of the test.

TEST FACILITY

BASF (2016b)

B.7. Eye Irritation – Rabbit

TEST SUBSTANCE

Assessed chemical

METHOD

OECD TG 405 Acute Eye Irritation/Corrosion (2012)

Species/Strain: Rabbit/New Zealand White/Hsdlf:NZW(SPF)

Number of Animals: 3F

Observation Period: 14 days

Remarks – Method: No significant protocol deviations.

RESULTS

Lesion	*Mean Score* Animal No.*			*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3			
Conjunctiva – Redness	2.0	2.0	1.7	2	< 14 days	0
Conjunctiva – Chemosis	1.3	2.0	1.7	2	< 14 days	0
Conjunctiva – Discharge	0	1.0	0.7	3	< 72 h	0
Corneal Opacity	0.7	1.0	0.3	1	< 7 days	0
Iridial Inflammation	0.7	0.7	0.0	1	< 72 h	0

* Calculated on the basis of the scores at 24, 48, and 72 hours for EACH animal

Remarks – Results

All animals showed moderate redness (grade 2), moderate chemosis (grade 2), severe discharge (grade 3) and slight cornea opacity (grade 1) at the 1 hour observation. Two animals also showed moderate iridial inflammation (grade 1) at the 1 hour observation.

Moderate redness and chemosis persisted in most animals at the 72 hour observation and the symptoms reduced to slight (grade 1) at the day 7 observation. The symptoms were resolved at the day 14 observation.

All animals showed severe discharge (grade 3) at 1 hour after application which regressed to grade 1 and 2 in two animals at 24 hours observation

	and then to slight discharge (grade 1) in two animals at 48 hours. The symptom was resolved at the 72 hour observation. Slight cornea opacity (grade 1) was observed in all animals at 1 and 24 hours after application, persisted in two animals at 24 hours and in one animal at the 72 hour observation and the symptom resolved at the day 7 observation. Moderate iritis (grade 1) was observed in two animals 1 hour after application and persisted until 48 hours. The animals were free of any iridial inflammation from 72 hour observation. Injected scleral vessels were observed in all animals at the 1 hour observation and the symptom persisted at the day 7 observation. All eyes appeared normal at the day 14 observation.
CONCLUSION	The assessed chemical is irritating to the eye (2A).
TEST FACILITY	Bioassay (2017c)

B.8. Skin Sensitisation – Guinea Pig, Buehler Test

TEST SUBSTANCE	Assessed chemical at 5% concentration
METHOD	OECD TG 406 Skin Sensitisation – Guinea Pig, Buehler Test (1992)
Species/Strain	Guinea pig/HsdDhl:DH,SPF
PRELIMINARY STUDY	Maximum non-irritating concentration: Topical: 2%
MAIN STUDY	
Number of Animals	Test Group: 20F Control Group: 10F
Vehicle	Deionised water
Positive Control	Not conducted in parallel with the test substance, but had been conducted previously in the test laboratory using 85% α-hexylcinnamaldehyde.
INDUCTION PHASE	Induction concentration: Topical: 5%
Signs of Irritation	In the test group, 12 animals showed discrete erythema (grade 1) after the first induction, while 14 animals showed discrete or moderate erythema (grade 1 or 2) after the second induction. 20 animals showed discrete or moderate erythema after the third induction. After the challenge 1 animal in total showed discrete erythema (grade 1).
CHALLENGE PHASE	
1st Challenge	Topical: 2%
2nd Challenge	Not conducted; no borderline results were observed from the 1st challenge
Remarks – Method	No significant protocol deviations Two preliminary tests were conducted. In the first preliminary test, 3 females were treated with 10%, 25%, 50% and 80% of the test substance at 4 sites. As erythema of varies grades were noted in majority of animals at all concentrations, a second preliminary test was performed A In the second preliminary test, 3 females were treated with 0.5%, 1%, 2% and 5% of the test substance at 4 sites. No signs of systemic toxicity were observed. All animals revealed site discrete erythema (grade 1) at hour 1 or from hour 1 until hour 24 after removal of the patch at the 5% concentration. At the lower concentrations no erythema was seen in the animals at any reading point. Therefore, a 5% and 2% test items preparation in deionized water were selected for the induction and challenge phases, respectively.

The main study was performed using a control group (10 animals) and test group (20 animals). The inductions were performed on days 0, 7 and 14 and challenge was carried out 14 days after the last induction.

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after:*			
		1st Challenge		*2nd Challenge**	
		24 h	*48 h*	*24 h*	*48 h*
Test Group	2%	1/20	0/20	-	-
Control Group	2%	0/10	0/10	-	-

*Not conducted

Remarks – Results

Discrete (grade 1) erythema was observed in 12 animals after the first induction and 12 animals showed discrete erythema and two animals moderate erythema (grade 2) after the second induction. After the third induction 13 animals showed discrete and 7 animals moderate erythema 24 hours after application

No local skin findings could be observed in the control group neither after the inductions nor the challenge. No unscheduled mortalities or signs of systemic toxicity were observed during the study period.

Normal bodyweight gain was observed in all animals.

CONCLUSION

There was no evidence of reactions indicative of skin sensitisation to the assessed chemical at 5% concentration under the conditions of the test.

TEST FACILITY

Bioassay (2017d)

B.9. Repeat Dose Oral Toxicity – Rat

TEST SUBSTANCE

Assessed chemical

METHOD

OECD TG 407 Repeated Dose 28-day Oral Toxicity Study in Rodents OK

Species/Strain: Rat/Wistar/Crl:WI(Han)

Route of Administration: Oral – diet

Exposure Information: Total exposure days: 28 days
Dose regimen: 7 days per week
Post-exposure observation period: nil

Vehicle: Nil

Remarks – Method: No dose range finding test was conducted.
No significant protocol deviations.

RESULTS

Group	*Number and Sex of Animals*	*Dose (mg/kg bw/day)*	*Mortality*
Control	5M/5F	0	0/10
Low Dose (1000 ppm)	5M/5F	85.6 (M), 90 (F)	0/10
Mid Dose (4,000 ppm)	5M/5F	337.7 (M), 346.4 (F)	0/10
High Dose (12,000 ppm)	5M/5F	1,057.1 (M), 1083.2 (F)	0/10

Mortality and Time to Death

No unscheduled mortalities were observed during the study.

Clinical Observations

General signs of systemic toxicity were not observed following clinical examination in males and females of all test groups testing up to the limit dose (12000 ppm). Minimal changes (<10% as compared to control) in mean body weights were also observed for male and female animals of all test groups 1-3 (1000, 4000 and 12000 ppm). Test substance-related adverse effects were not observed with regards to functional observational battery as well as measurement of motor activity tests.

Laboratory Findings – Clinical Chemistry, Haematology, Urinalysis

Females at the highest dose level (12000 ppm) had marginally but statistically significant decreased haemoglobin (8 mmol/L) and haematocrit (0.373 L/L) values without any changes of the red blood cell indices, indicated a normochromic-normocytic anaemia. These values were below the historical control ranges for haemoglobin (8.1-9.1 mmol/L) and haematocrit (0.377-0.412 L/L). No treatment-related changes among urinalysis parameters were observed.

Effects in Organs

Test-substance related adverse findings were not noted in any of the treatment groups.
Statistically significant increase in relative heart weight in low and mid dose females were observed. As no adverse histopathological findings were observed, this effect is not considered to be toxicologically significant.

Remarks – Results

Two male animals of test group 3 showed minimal centrilobular hepatocellular hypertrophy in the liver, that was regarded as treatment-related but not adverse. The lack of periportal fatty change in test group 3 males in comparison to control animals was related to the slightly decreased terminal body weight (not statistically significant) in these animals. It was regarded as treatment-related but not adverse.

Male animals of test groups 2 and 3 showed a minimally increased severity of inflammatory cell infiltrates in the glandular stomach. The increased severity of inflammatory cell infiltrates was regarded as treatment-related but not adverse, since there were no additional degenerating changes in the mucosal or submucosal layer observed.

CONCLUSION

The No Observed Adverse Effect Level (NOAEL) was established as 346 mg/kg bw/day (4,000 ppm) in females, based on reduction in haemoglobin and haematocrit levels and 1,057 mg/kg bw/day (12,000 ppm) in males, based on no toxicologically relevant adverse effects at this dose level.

TEST FACILITY	BASF (2018)

B.10. Genotoxicity – Bacteria

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 471 Bacterial Reverse Mutation Test (1997) Plate incorporation procedure (test 1) and pre incubation procedure (test 2)
Species/Strain	*Salmonella typhimurium*: TA1535, TA1537, TA98, TA100, *Escherichia coli*: WP2uvrA
Metabolic Activation System	S9 mix from phenobarbital/β-naphthoflavone induced rat liver
Concentration Range in Main Test	a) With metabolic activation: 33, 100, 333, 1,000, 2,500 and 5,000 µg/plate b) Without metabolic activation: 33, 100, 333, 1,000, 2,500 and 5,000 µg/plate
Vehicle	Dimethyl sulfoxide (DMSO)
Remarks – Method	No preliminary test was conducted. Vehicle and positive control studies were conducted in parallel with the main study. Negative controls: DMSO Positive control: With metabolic activation: 2-aminoanthracene (TA 1535, TA 100, TA 1537, TA 98 and WP2uvrA) Without metabolic activation: *N*-methyl-*N'*-nitro-*N*-nitrosoguanidine TA 1535 and TA 100), 4-nitro-o-phenylenediamine (TA 98), 9-aminoacridine (TA 1537) and 4-nitroquinoline-*N*-oxide (WP2uvrA).

No significant protocol deviations.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	Not tested	≥ 2,500	≥ 5,000	Negative
Test 2	-	≥ 2,500	≥ 5,000	Negative
Present				
Test 1	Not tested	≥ 2,500	≥ 5,000	Negative
Test 2	-	≥ 5,000	≥ 5,000	Negative

Remarks – Results: No biologically relevant increases in revertant colony numbers of any of the tester strains were observed during the test in either the presence or absence of metabolic activation.

The positive controls induced a distinct increase of revertant colonies during the study indicating the validity of the test system.

CONCLUSION: The assessed chemical was not mutagenic to bacteria under the conditions of the test.

TEST FACILITY: BASF (2016e)

B.11. Genotoxicity – *In Vitro* Gene Mutation Test in Chinese Hamster Ovary Cells (HPRT LOCUS ASSAY)

TEST SUBSTANCE: Assessed chemical

METHOD: OECD TG 476 *In vitro* Mammalian Cell Gene Mutation Test using the Hprt and xprt genes"

Species/Strain: *Chinese hamster*
Cell Type/Cell Line: Chinese hamster ovary (CHO) cell line
Metabolic Activation System: S9 mix from phenobarbital/β-naphthoflavone induced rat liver
Vehicle: Culture medium
Remarks – Method: Negative control: culture medium
Positive control:
Without S9: ethyl methanesulfonate (EMS)
With S9: 7,12-dimethylbenz[a]anthracene (DMBA)

In a preliminary test, CHO cells were treated with the test substance at 19.5 to 5,000.0 µg/mL for 4 hours with or without metabolic activation.

Minor protocol deviations.

Metabolic Activation	*Test Substance Concentration (µg/mL)*	*Exposure Period*	*Expression Time*	*Selection Time*
Absent				
Test 1	0*, 12.5*, 25.0*, 50.0*, 100.0*, 200.0*, 400.0 and 600.0	4 hours	3 days	6-7 days
Test 2	0*, 12.5*, 25.0*, 50.0*, 100.0*, 200.0*, 400.0* and 600.0	4 hours	3 days	6-7 days
Present				
Test 1	0*, 9.4, 18.8*, 37.5*, 75.0*, 150.0*, 300.0* and 600.0	4 hours	3 days	6-7 days
Test 2	0*, 9.4, 18.8*, 37.5*, 75.0*, 150.0*, 300.0* and 600.0	4 hours	3 days	6-7 days

*Cultures selected for metaphase analysis

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/mL) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	≥ 312.5	≥ 400	≥ 600	Negative
Test 2	-	≥ 600	≥ 600	Negative
Present				
Test 1	≥ 312.5	≥ 400	≥ 600	Negative
Test 2	-	≥ 300	≥ 600	Negative

Remarks – Results

In the preliminary toxicity test up to 5,000 µg/mL, the test substance induced evidence of toxicity at ≥ 312.5 µg/mL (3.4% relative cloning efficiency at a concentration of 312.5 µg/mL without metabolic activation and 1.8% cloning efficiency at 312.5 µg/mL with metabolic activation) at an exposure period of 4 hours.

Due to strong cytotoxicity at concentrations of 400 to 600 µg/mL both with and without metabolic activity in both Tests 1 and 2, the culture were discontinued.

CONCLUSION OK

The assessed chemical was not a mutagenic in the HPRT locus assay using Chinese hamster ovary cells under the conditions of the test.

TEST FACILITY

BASF (2016d)

B.12. Genotoxicity – *In Vitro* Micronucleus Assay in V79 Cells

TEST SUBSTANCE

Assessed chemical

METHOD

OECD TG 476 *In vitro* Mammalian Cell Micronucleus Test (2014)

Species/Strain: *Chinese hamster*

Cell Type/Cell Line: Chinese hamster V79 cell line

Metabolic Activation System: S9 mix from phenobarbital/β-naphthoflavone induced rat liver

Vehicle: Culture medium

Remarks – Method:
Negative control: culture medium
Positive control:
Without S9: ethyl methanesulfonate
With S9: cyclophosphamide

In a preliminary test, V79 cells were treated with test substance at 39.1 to 5,000.0 µg/mL for 4 and 24 hours without metabolic activation and 4 hours with metabolic activation.
Severe cytotoxicity occurred in the first experiment without S9 mix and therefore did not fulfil the requirements of the current OECD guidelines. A repeat experiment was therefore performed.

Metabolic Activation	*Test Substance Concentration (µg/mL)*	*Exposure Period*	*Recovery Time*	*Harvest Time*
Absent				
Test 1	0, 31.3, 62.5, 125.0, 250.0, 500.0 and 1000.0	4 hours	20 hours	24 hours
Test 2	0*, 6.3, 12.5, 25.0, 50.0*, 100.0* and 200.0*	4 hours	-	24 hours
Test 3	0*, 6.3, 12.5, 25.0, 50.0*, 100.0* and 200.0*	24 hours	20 hours	24 hours
Present				
Test 1	0*, 31.3, 62.5*, 125.0*, 250.0*, 500.0* and 1000.0	4 hours	20 hours	24 hours

Test 2	0*, 25.0, 50.0*, 100.0*, 200.0*, 400.0* and 800.0	4 hours	40 hours	44 hours

*Cultures selected for metaphase analysis

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/mL) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	≥ 312.5	≥ 62.5	≥ 250	Negative
Test 2	-	> 200	≥ 200	Positive
Test 3	-	> 200	≥ 200	Equivocal
Present				
Test 1	≥ 312.5	≥ 500	≥ 250	Negative
Test 2	-	≥ 400	≥ 200	Negative

Remarks – Results

A statistically significant but not dose related increase in micronucleated cells was observed at 400 µg/mL in the 2nd experiment with metabolic activation. This increase was above 95% control limits of the distribution of the historically controlled negative values. However, the relative population doubling was reduced to 30.2% compared to vehicle control at this test group. The study authors therefore considered this finding as not biologically irrelevant due to severe cytotoxicity and strong test substance precipitation in culture medium.

The result obtained in test 3, without metabolic activation at 100 µg/m (1.1% micronuleated cells) was slightly above the 95% historical negative control values (0.0-1.0%). The value, however, was close to the respective negative control value (0.8% micronucleated cells) and therefore, it was not statistically significant. The study authors therefore considered this observation was not biologically relevant.

Positive and negative controls performed as expected.

CONCLUSION

The assessed chemical was not clastogenic to V79 cells treated *in vitro* under the conditions of the test.

TEST FACILITY

BASF (2016c)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready Biodegradability

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 301 B Ready Biodegradability: CO2 Evolution Test
Inoculum	Activated sludge
Exposure Period	28 days
Auxiliary Solvent	None
Analytical Monitoring	TOC
Remarks – Method	Aniline was used as a reference substance. A toxicity control was also conducted.

RESULTS

Test Substance		*Aniline*		*Toxicity control*	
Day	*% Degradation*	*Day*	*% Degradation*	*Day*	*% Degradation*
4	18	4	33	4	31
11	38	11	77	11	57
14	46	14	83	14	62
28	73	28	91	28	77

Remarks – Results	All validity criteria were met. The inorganic carbon content in the test solutions at the start of the test was < 1 mg/L, the difference in extremes at the end of the test was 2%, and the CO_2 evolution of the inoculum blank was 38 mg CO_2/L. The toxicity control reached the pass level by day 7 and is therefore not considered inhibitory to the inoculum.
CONCLUSION	The test substance is readily biodegradable.
TEST FACILITY	BASF (2013)

C.2. Ecotoxicological Investigations

The assessed chemical has a measured water solubility of 63.35 g/L. However, it is a surfactant and the measured value is likely to be an overestimate of the true water solubility, as the measured value may include aqueous dispersions.

C.2.1. Acute Toxicity to Fish

TEST SUBSTANCE	Assessed chemical
METHOD	OECD TG 203 Fish, Acute Toxicity Test - Semi static
Species	Rare Minnow (*Gobiocypris rarus*)
Exposure Period	96 h
Auxiliary Solvent	None
Water Hardness	None
Analytical Monitoring	UPLC-MS analysis
Remarks – Method	Based on a range finding study, test concentrations (detailed below) were prepared as Water Accommodated Fractions (WAFs). WAFs were prepared by adding the required amount of the test substance in test water and stirring for about 30 min. Test solutions were renewed after 48 hours. A positive control (potassium dichromate) was used for annual quality assurance to evaluate fish quality and test conditions.

RESULTS

Concentration (mg/L)		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*1 h*	*24 h*	*48 h*	*72 h*	*96 h*
Control	-	7	0	0	0	0	0
1.2	-	7	0	0	0	0	0
2.2	-	7	0	0	0	0	0
4.0	-	7	0	0	0	0	0
7.0	-	7	0	5	5	5	6
12.0	-	7	0	6	7	7	7

LL50 5.72 mg/L at 96 hours

Remarks – Results All validity criteria for the study were met. The dissolved oxygen concentration was ≥ 80% of air saturation value throughout the test.
Since the measured concentrations in each group varied less than 20% during each renewal period, the nominal loading rates were used. The 96 h LL50 with 95% confidence limits were calculated using Spearman-Karber method. The 96 h LC50 for *Gabiocypris rarus* exposed to potassium dichromate was within the range of expected responses.

CONCLUSION The test substance is acutely toxic to fish.

TEST FACILITY BSAL (2018)

TEST SUBSTANCE Assessed chemical

METHOD OECD TG 203 Fish, Acute Toxicity Test -Semi static
Species Zebra fish (*Danio rerio*)
Exposure Period 96 h
Auxiliary Solvent None
Water Hardness 10 - 250 mg $CaCO_3$/L
Analytical Monitoring TOC
Remarks – Method Based on a range finding study, test concentrations (detailed below) were prepared from dilution of a stock solution and filtered to obtain water soluble fractions (WSFs) from water accommodated fractions (WAFs). Nominal loading levels of WSFs were used in the test and renewed after 24 hours.

RESULTS

Concentration (mg/L)		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*1 h*	*24 h*	*48 h*	*72 h*	*96 h*
Control	-	7	0	0	0	0	0
6.25	-	7	0	0	0	0	0
12	-	7	0	0	0	0	0
25	-	7	0	2	5	7	7
50	-	7	0	7	7	7	7
100	-	7	0	7	7	7	7

LL50 17.7 mg/L at 96 hours

Remarks – Results All validity criteria for the study were met. There was no mortality in the control. The dissolved oxygen concentration was ≥ 80% of air saturation value throughout the test. Since no specific analysis of the test item was performed, all effect levels were based on the nominal loading of the test item. The 96 h LL50 was 17.7 (12.5 – 25) mg test item/L (geometric mean of LL100/LL0 based on nominal test item nominal loadings. The LL0 and

LL100 after 96 h were 12.5 and 25 mg test item/L (nominal test item loadings).

CONCLUSION The test substance is acutely harmful to fish.

TEST FACILITY Noack (2017)

C.2.2. Acute Toxicity to Aquatic Invertebrates

TEST SUBSTANCE Assessed chemical

METHOD OECD TG 202 Daphnia sp. Acute Immobilisation Test and Reproduction Test – semi-static

Species *Daphnia magna*
Exposure Period 48 hours
Auxiliary Solvent None
Water Hardness 160 - 180 mg $CaCO_3$/L
Analytical Monitoring Total Organic Carbon
Remarks – Method Based on a range finding study, test concentrations (detailed below) were prepared from dilution of a stock solution and filtered to obtain water soluble fractions (WSFs) from water accommodated fractions (WAFs). Test solutions were renewed after 24 hours.
A positive control (potassium dichromate) was used for monthly quality assurance to evaluate the test conditions.

RESULTS

Concentration (mg/L) Nominal loading	*Number of D. magna*	*Number Immobilised*	
		24 h	*48 h*
Control	20	0	0
6.25	20	0	0
12.5	20	0	0
25	20	0	0
50	20	2	3
100	20	5	11

EL50 93 mg/L at 48 hours
Remarks – Results All validity criteria were met. Dissolved oxygen was maintained at > 6.69 mg/L, pH was maintained between 7.65 and 7.8 and temperature was maintained at 20°C ± 1°C. The EC50 for potassium dichromate was 1.95 which is within the expected range. The EC50 was calculated based on nominal concentrations using sigmoidal dose-response regression.

CONCLUSION Test substance is harmful to aquatic invertebrates.

TEST FACILITY Noack (2016)

C.2.3. Algal Growth Inhibition Test

TEST SUBSTANCE Assessed chemical

METHOD OECD TG 201 Alga, Growth Inhibition Test

Species *Raphidocelis subcapitata*
Exposure Period 72 hours
Concentration Range Nominal: 0.1 – 228.8 mg/L
Auxiliary Solvent None
Analytical Monitoring TOC
Remarks – Method Based on a range finding study, test concentrations were prepared from dilution of a stock solution and filtered to obtain Water Accommodated Fractions (WAF).

RESULTS

Growth rate		*Yield*	
ErL50 (mg/L)	*NOEL (mg/L)*	*EyL50 (mg/L)*	*NOEL (mg/L)*
116	50	54.9	50

Remarks – Results: All validity criteria were met. The control cell density increased by a factor of 95.3, the mean coefficient of variation for section-by-section specific growth was 27.8% and the coefficient of variation for the average specific growth rates was 2.3%.

CONCLUSION: Test substance is harmful to algal growth.

TEST FACILITY: Hydrot (2017)

C.2.4. Inhibition of Microbial Activity

TEST SUBSTANCE: Assessed chemical

METHOD: OECD TG 209 Activated Sludge, Respiration Inhibition Test
- Inoculum: Activated sludge
- Exposure Period: 3 hours
- Concentration Range: Nominal: 62.5 - 1000 mg/L
- Remarks – Method: 3,5-dichlorophenol was used as a reference substance.

RESULTS
- EC50: >1000 mg/L
- EC10: 260 mg/L
- Remarks – Results: All validity criteria were met. The coefficient of variation of the oxygen consumption of the blank controls was 6.2%, the mean oxygen uptake of the blank controls was 35 mg/g×h and the EC50 of 3,5-dichlorophenol was 6.8 mg/L

CONCLUSION: The test substance was not harmful to microbial respiration.

TEST FACILITY: BASF (2016f)

C.2.5. Soil Microorganisms: Nitrogen transformation test

TEST SUBSTANCE: Assessed chemical

METHOD: OECD TG 216 Soil Microorganisms: Nitrogen Transformation Test
- Test system: Natural soil
- Exposure Period: 28 days
- Concentration Range: Nominal: 62.5 - 1000 mg/L
- Remarks – Method: Based on a range finding study, test concentrations were prepared from dilution of a stock solution.

RESULTS
- EC50: > 1000 mg/L
- Remarks – Results: All validity criteria were met. The variation between replicate control samples was ≤ 3.2% across the 28 day testing period.

CONCLUSION: The test substance was not harmful to microbial nitrification.

TEST FACILITY: BASF (2019)

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