File No: STD/1475

July 2013

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

Alkanolamine reaction product with carbon dioxide

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 Ageing, and conducts the risk assessment for public health and occupational health and safety. The assessment of environmental risk is conducted by the Department of Sustainability, Environment, Water, Population and Communities.

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:

Street Address:	Level 7, 260 Elizabeth Street, SURRY HILLS NSW 2010, AUSTRALIA.
Postal Address:	GPO Box 58, SYDNEY NSW 2001, AUSTRALIA.
TEL:	+ 61 2 8577 8800
FAX	+ 61 2 8577 8888
Website:	www.nicnas.gov.au

Director
NICNAS

TABLE OF CONTENTS

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/1475	BP Australia Pty Ltd	Alkanolamine reaction product with carbon dioxide	Yes	< 50 tonnes per annum	Component of industrial metal working fluid systems.

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*
Acute Toxicity (Category 4)	H302 – Harmful if swallowed
Eye Irritation (Category 2A)	H319 – Causes serious eye irritation

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
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 Aquatic Toxicity (Category 3)	H402 – Harmful to aquatic life

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.

Recommendations

REGULATORY CONTROLS
Hazard Classification and Labelling

- The notified chemical should be classified as follows:
  - Acute Toxicity (Category 4): H302 – Harmful if swallowed;
  - Eye Irritation (Category 2A): H319– Causes serious eye irritation

Classification of products/mixtures containing the notified chemical should be considered based on the concentration of the notified chemical present.

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 notified chemical:
  - Local ventilation systems, where possible

- 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:
  - Avoid contact with skin and eyes
  - Avoid breathing mist/vapours
  - A shower and eyewash station should be available

- 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:
  - Coveralls
  - Impervious gloves
  - Goggles
  - Respiratory protection if ventilation is inadequate

  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.

Disposal

- The notified chemical should be disposed of to landfill.

Storage

- The handling and storage of the notified 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 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(2) of the Act; if
- the function or use of the chemical has changed from a component of metal working fluid systems or is likely to change significantly;
- the amount of chemical being introduced has increased from 50 tonnes per annum, 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.

(Material) Safety Data Sheet
The (M)SDS of products 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)
BP Australia Pty Ltd (ABN: 53 004 085 616)
Level 16, 717 Bourke St
Melbourne 3008

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 and import volume.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: acute oral toxicity, acute dermal toxicity and repeat dose toxicity.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
United States of America (2006)

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Alkanolamine reaction product with carbon dioxide
BOOST WP 45 (product containing the notified chemical)

MOLECULAR WEIGHT
< 500 Da

ANALYTICAL DATA
Reference NMR spectra were provided.

3. COMPOSITION

DEGREE OF PURITY > 50%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS
The notified chemical contains an impurity at a concentration of > 25%, which may result in harmful effects via inhalation, in contact with skin and if swallowed, and may cause burns.

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20 °C AND 101.3 kPa: Pale amber coloured viscous liquid.

Property	Value	Data Source/Justification
Pour Point	273 ± 3 K (~0 °C)	Measured
Boiling Point	Decomposes at 376 K (~103 °C) at 100.84 kPa	Measured
Density	1.27×10^3 kg/m^3 at 20.0 ± 0.5 °C	Measured
Vapour Pressure	8.2×10^{-4} kPa at 25 °C	Measured
Water Solubility	Miscible in water at 20 °C	Measured
Hydrolysis as a Function of pH	Not determined	Contains hydrolysable functionalities and is expected to decompose under the environmental conditions.
Partition Coefficient (n-octanol/water)	log Pow = -1.78 at 22.5 ± 0.5°C	Measured
Adsorption/Desorption	log K_{oc} = -0.85	Estimated
Dissociation Constant	pKa = 5.31 ± 0.41	Calculated
Flash Point	No flash point below decomposition temperature	Measured
Autoignition Temperature	> 400 °C	Measured
Explosive Properties	Predicted negative	Does not contain any functional groups that would imply explosive properties
Oxidising Properties	Predicted negative	Does not contain any functional groups that would imply oxidative properties

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

Reactivity
The notified chemical is not expected to react with water or in air; however, it is sensitive to pH and temperature changes.

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 not be manufactured in Australia. The notified chemical will be imported as a component of metal working fluids at concentrations of 2 – 10%.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	< 50	< 50	< 50	< 50	< 50

PORT OF ENTRY
Melbourne and Sydney

IDENTITY OF RECIPIENTS

BP Australia Pty Ltd and/or Australasian Lubricants Manufacturing Company Pty Ltd (ALMC)

TRANSPORTATION AND PACKAGING
The notified chemical (at 2 – 10% concentration) will be imported by sea in 200 L drums and transported to the end-use customers' facilities for reformulation into metal working fluids. All products containing the notified chemical will be transported by either road or rail within Australia.

USE
The notified chemical will be used as a component of industrial metal working fluid systems.

OPERATION DESCRIPTION
The notified chemical will not be manufactured within Australia.

End use
The products containing the notified chemical will not be sold to the public.

Following transportation to the end use customers, the imported metal working fluids (containing 2 – 10% of the notified chemical) will be diluted with water and other components before filling into individual metal working machines or centralised metal working fluid tanks (sump size normally in the range of 20,000 – 50,000 L). The concentration of the notified chemical in the diluted metal working fluids is anticipated to be 0.1 – 1.0%. These diluted fluids will then be used in various metal working processes.

Any waste generated during the dilution and use of the metal working fluids and any spent metal working fluids are expected to be collected for disposal by a licensed waste disposal contractor.

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 storage	2-4	15-60
Quality control	1-2	40-60
End use	7-8	20-250
Disposal	1-2	8-50

EXPOSURE DETAILS
Transport and storage
Transport and storage workers are not expected to be exposed to the notified chemical except in the unlikely event of an accidental rupture of containers. In the unlikely event of a spill, appropriate personal protective equipment (PPE) is expected to be worn by clean up staff.

End users
Worker exposure to the notified chemical at ≤ 10% concentration is possible during dilution (blending), filling, transfer, maintenance and quality control operations and at ≤ 1% in end use operations. The main routes of exposure would be dermal and ocular. Inhalation exposure to the notified chemical at ≤ 1% concentration is also possible during end use of metal working fluids. Exposure is expected to be minimised by the use of adequate local ventilation systems. In addition, PPE is expected to be worn by all workers, including coveralls, impervious gloves, eye protection and if ventilation is insufficient, suitable respiratory protection.

6.1.2. Public Exposure
The notified chemical is expected to be used in industrial settings only. Therefore, given the proposed use pattern, public exposure is not expected.

6.2. Human Health Effects Assessment

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

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity*	LD50 ≥ 1089 mg/kg bw; harmful
Rat, acute dermal toxicity*	LD50 = [2504, 2881] mg/kg bw; low toxicity
Skin irritation (in vitro skin irritation)	non-irritating
Skin irritation (in vitro skin corrosion)	non-corrosive
Rabbit, skin irritation	slightly irritating
Eye irritation (in vitro)	non-irritating
Rabbit, eye irritation	slightly irritating
Guinea pig, skin sensitisation – non-adjuvant test.	no evidence of sensitisation
Rat, repeat dose oral toxicity 28 days*	NOAEL = 770 mg/kg bw/day
Mutagenicity – bacterial reverse mutation	non mutagenic
Genotoxicity – in vitro chromosome aberration test	non genotoxic

*Data on the parent alkanolamine (IUCLID, 2008).

Toxicokinetics, metabolism and distribution.
Based on the low molecular weight of the chemical (< 500 Da), dermal absorption may occur; however, the extent of absorption may be limited by the chemical being a salt (water miscible; log Kow = -1.78). At low pH (as in the stomach), the notified chemical is expected to have dissociated, with the predominant species present being the parent alkanolamine.

Acute toxicity.
No acute toxicity study reports were provided for the notified chemical. However, information on the acute oral and dermal toxicity of an acceptable analogue of the notified chemical (the parent alkanolamine) was available (IUCLID, 2008).

In an acute oral toxicity study on the parent alkanolamine, 40 rats (5/sex/dose) were treated with ~254.5 – 2036 mg/kg bw test substance by gavage. Additionally 2 males were treated with 4072 mg/kg bw test substance. There were numerous deaths reported during the course of the study including all high dose animals within 24hrs of dosing. General signs of toxicity were noted at mid and high treatment doses, including sluggishness, piloerection, red crusting of the perinasal and periocular fur and emaciation. Surviving animals generally recovered but emaciation was noted to persist in females and 1 male until sacrifice (at 14 days after dosing). Numerous lesions were noted at necropsy in animals treated with mid and high doses including in the kidneys, GI tract and lungs. The acute oral LD50 for the parent alkanolamine was determined to be between 1018 and 2036 mg/kg bw (reported as 1089 and 1211 mg/kg bw for females and males, respectively) (IUCLID, 2008). In addition, it is noted that the parent alkanolamine is classified as harmful via the oral route (HSIS; R22 – Harmful if swallowed). Based on the available information the notified chemical is also expected to be harmful via the oral route.

In an acute dermal toxicity study on the parent alkanolamine, 30 rabbits (5/sex/dose) were treated with ~1018, 2036 and 4072 mg/kg bw test substance for 24 hours (occlusive conditions). Multiple deaths were reported during the study period of 14 days. However, there were no deaths recorded at the lowest dose tested. Local signs of irritation were noted in animals of all treatment groups and included persisting erythema, oedema, necrosis ecchymosis and some ulceration. Signs of systemic toxicity, including emaciation and sluggishness, were only noted in the majority of animals treated with ≥ 2036 mg/kg bw. Numerous lesions were noted at all treatment doses at necropsy including in the kidneys, GI tract and lungs. The acute dermal LD50 for the parent alkanolamine was determined to be between 2036 and 4072 mg/kg bw (reported as 2504 and 2881 mg/kg bw for males and females, respectively) (IUCLID, 2008). The parent alkanolamine is classified as harmful via the dermal route (HSIS; R21 – Harmful in contact with skin; range of LD50 values reported in IUCLID, 2000, study details unavailable). However, skin irritation studies on the notified chemical (see below) indicate that it is only slightly irritating to the skin and eyes of rabbits, whereas the parent chemical is classified as corrosive (HSIS – R34 – causes burns). Therefore, considering the composition of the notified chemical relative to the parent alkanolamine, there is some uncertainty regarding the relevance of the acute dermal classification of the parent alkanolamine to the notified chemical. However, the results of studies conducted on the parent alkanolamine are expected to represent a worst case scenario and in the absence of acute dermal data on the notified chemical, the notified chemical is considered to be of low acute toxicity via the dermal route.

There was no data provided on the acute inhalation toxicity of the notified chemical. The parent alkanolamine is classified as harmful via the inhalation route (HSIS; R20 – Harmful by inhalation). However, there are differences in the vapour pressures between the notified chemical and parent alkanolamine and, as noted above, the parent alkanolamine is a corrosive substance.

Irritation and sensitisation.
The notified chemical was slightly irritating to the skin and eyes of rabbits. Very slight erythema was noted on the skin of 1/3 rabbits treated with the test substance 1 hour after patch removal, with the skin appearing normal after 24 hours. Slight to moderate iridial and conjunctival effects were noted in the eyes of 2 rabbits treated with the test substance, with the eyes also appearing normal within 7 days following instillation. Negative results were obtained in *in vitro* tests for skin irritation/corrosion and eye irritation.

The notified chemical is sensitive to pH, being expected to dissociate in acidic conditions, with the predominant species present being the parent alkanolamine. The irritation scores in the in vivo studies were narrowly insufficient to warrant classification of the notified chemical as an irritant. However, the notifier has indicated that the notified chemical should be considered as being irritating to the eyes.

A Buehler sensitisation study (50% induction concentration; 10% challenge concentration) on the notified chemical indicated no evidence of skin sensitisation. The 10% challenge concentration was selected based on the observation of slight irritation in 2/3 animals in a preliminary study, when treated at 25% concentration.

Repeated Dose Toxicity.
No repeated dose toxicity data were provided on the notified chemical. Multiple repeated dose toxicity studies on the parent alkanolamine have been reported (e.g. IUCLID, 2008). In one repeated dose feeding study on the parent alkanolamine, groups of 10 male rats were administered 0.01, 0.1 and 1.0% (equivalent to 770 mg/kg bw/day) test substance via the diet for 32 days. There were no deaths reported during the study, and were no treatment related changes noted for body weight gain, diet efficiency, feed consumption or histopathology at any treatment level. Average absolute and relative liver weights were significantly increased in animals treated with feed containing 0.01 and 0.1% test substance compared to controls, however, there was no significant increase noted in animals treated with 1.0% test substance. The NOAEL for the parent alkanolamine was established as 1% (770 mg/kg bw/day) in this study (IUCLID, 2008). In the absence of relevant data for the notified chemical, as a worst case scenario, the notified chemical is expected to exhibit repeated dose toxicity to rats, at a similar level as the parent alkanolamine chemical.

Mutagenicity/Genotoxicity.
Bacterial reverse mutation and *in vitro* chromosomal aberration studies on the notified chemical were negative. Based on the information provided, the notified chemical is not considered to be mutagenic/genotoxic.

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***
Acute Toxicity (Category 4)	H302 – Harmful if swallowed
Eye Irritation (Category 2A)	H319 – Causes serious eye irritation

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
R36: Irritating to eyes

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety
The notified chemical is an acute oral toxicant, is irritating to the eyes, and may be harmful via the inhalation route.

Workers may be exposed to the notified chemical (at ≤ 10% concentration) during transfer of the solution

containing the notified chemical from transport containers to mixing vessels and during general maintenance operations. There may also be exposure during use of diluted metal working fluids (at ≤ 1% concentration).

The primary risks associated with worker exposure will be due to the systemic toxicity and irritating nature of the chemical. However, dermal and ocular exposure to the notified chemical is expected to be minimised by the wearing of PPE, including gloves, coveralls, and eye protection. Thus the risk of irritation is not considered to be unreasonable. Ingestion is unlikely under the proposed use scenario and thus the risk of acute oral toxicity is not considered unreasonable. Exposure via inhalation is possible during end use of the metal work fluids containing ≤ 1% concentration of the notified chemical but is expected to be lowered by the use of adequate local ventilation systems and respiratory protection Provided that control measures are in place to minimise worker exposure, including the use of local ventilation and PPE, the risk to the health of workers from use of the notified chemical is not considered to be unreasonable.

6.3.2. Public Health

The notified chemical is only intended for use in industrial settings by trained workers. The public may only be exposed to the notified chemical in the unlikely event of an accident during transport. Therefore, when used in the proposed manner, the risk to public health from the notified chemical 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 will be imported into Australia as component of concentrated metal working fluids. Products containing the notified chemical will be diluted with water and other components to form the final products by end-use customers. The blending is expected to take place in fully-contained, industrial facilities. Spills and leaks during transport, storage and blending are expected to be very low. Any waste metal working fluids containing the notified chemical are expected be collected for disposal by an approved waste management company.

RELEASE OF CHEMICAL FROM USE

Metal working fluids containing the notified chemical will be circulated through contained systems until they are spent. Spent metal working fluids are expected to be collected for disposal by an approved waste management company.

RELEASE OF CHEMICAL FROM DISPOSAL

Residues in empty containers, spills and spent metal working fluids are expected to be collected for disposal by an approved waste management company. The waste metal working fluids are likely to be finally disposed of to sewer via wastewater treatment at approved waste management company sites.

7.1.2. Environmental Fate

The notified chemical is not expected to partition to the air compartment based on the low vapour pressure (0.082 Pa). The majority of notified chemical is expected to be released to wastewater streams from the discharge of the spent metal working fluids. The wastewater is expected to be collected and treated by an approved waste management company before release to public sewers. During the wastewater treatment processes at the waste management site/s or sewage treatment plant/s, most of the notified chemical is expected to be removed by degradation given the notified chemical is readily biodegradable (100% over 28 days). In addition, the notified chemical is expected to hydrolyse under the environmental conditions (pH range of 4-9). Despite the expected efficient removal during wastewater treatment processes, a small amount of notified chemical may be released to receiving waters. However, the notified chemical is expected to disperse and degrade. Bioaccumulation is not expected due to its high water solubility and low water/octanol partition coefficient (log Pow = -1.78). Sludge from the wastewater treatment plant/s which may contain limited amount of the notified chemical is expected to be disposed of to landfill or applied to agricultural soils.

Notified chemical in landfill or soil is expected to mobile based on its estimated low soil adsorption coefficient (log Koc = -0.85). However, in landfill, soil and water, the notified chemical is expected to rapidly degrade into water, and oxides of carbon and nitrogen. For the details of the environmental fate study please refer to Appendix C.

7.1.3. Predicted Environmental Concentration (PEC)

Wastewater streams receiving the spent notified chemical may be directed to sewers. Therefore, under a worst case scenario, it is assumed that 100 % of the total import volume of the notified chemical will be discharged into sewers over 260 days per year corresponding to release only on working days. It is estimated by SimpleTreat (EC, 2003) that 87% of the notified chemical is removed from influent via biodegradation during sewage treatment processes. The predicted environmental concentration (PEC) can be estimated as outlined below.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	50,000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	50,000	kg/year
Days per year where release occurs	260	days/year
Daily chemical release:	192.31	kg/day
Water use	200	L/person/day
Population of Australia (Millions)	22.613	million
Removal within STP	87%	Mitigation
Daily effluent production:	4,523	ML
Dilution Factor - River	1	
Dilution Factor - Ocean	10	
PEC - River:	5.53	µg/L
PEC - Ocean:	0.55	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 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 5.528 µg/L may potentially result in a soil concentration of approximately 36.85 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 184.3 µg/kg and 368.5 µg/kg, respectively.

7.2. Environmental Effects Assessment

The results from ecotoxicological investigations conducted on the notified chemical are summarised in the table below. Details of these studies can be found in Appendix C.

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	LC50 (96 hours) > 100 mg/L	Not harmful to fish
Daphnia Toxicity	EC50 (48 hours) = 32 mg/L	Harmful to aquatic invertebrates
Algal Toxicity	E_rC50 (72 hours) = 39 mg/L	Harmful to algae

Based on the acute toxicity for daphnia and algae, the notified chemical is formally classified as "Acute Category 3: Harmful to aquatic life" under the Globally Harmonised System of Classification and Labelling of Chemicals (GHS; United Nations, 2009). The notified chemical is readily biodegradable and not expected to bioaccumulate. Based on the available acute endpoints for the notified chemical, it is not formally classified under GHS for long-term hazard.

7.2.1. Predicted No-Effect Concentration

The endpoint (48 hours EC50 = 32 mg/L) for the most sensitive species (daphnia) from the reported results is used to calculate the predicted no-effect concentration (PNEC). An assessment factor of 100 was used as the endpoints for three tropic levels are available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
EC50 (Invertebrates).	32	mg/L
Assessment Factor	100	
PNEC:	320	µg/L

7.3. Environmental Risk Assessment

Risk Assessment	***PEC µg/L***	***PNEC µg/L***	***Q***
Q - River:	5.53	320	0.017
Q - Ocean:	0.55	320	0.002

The Risk Quotients (Q = PEC/PNEC) for the worst case scenario have been calculated to be < 1 for the river and ocean compartments. Although the notified chemical may be released into waterways, it is not expected to pose a risk to the aquatic environment as ecotoxicologically significant concentrations are unlikely to be reached under this assessed scenario. The notified chemical is expected to rapidly degrade in the environment and bioaccumulation is not expected. Therefore, 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.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Pour Point 273 ± 3 K (~0 °C)

Method OECD TG 102 Melting Point/Melting Range.
Remarks The experiment was run in duplicate using a series of baths (48 to -18 °C) to cool the sample.
Test Facility Harlan (2010a)

Boiling Point Decomposes at 376 K (~103 °C) at 100.84 kPa

Method OECD TG 103 Boiling Point.
Remarks Determined using differential scanning calorimetry (DSC).

The experiment was run using both manually pierced crucibles and pre-perforated crucibles under both air and nitrogen atmospheres. The study authors indicated that the data and observations recorded when determining the flash point (see below) were consistent with the notified chemical having decomposed into the starting components (at ~103 °C, followed by the subsequent boiling of the remaining components. After the experiment, a pale yellow residue (negligible amount) remained in the sample container.
Test Facility Harlan (2010a)

Density 1.27×10^3 kg/m^3 at 20.0 ± 0.5 °C

Method OECD TG 109 Density of Liquids and Solids.
Remarks The density was determined using a glass pycnometer.
Test Facility Harlan (2010a)

Vapour Pressure 8.2×10^{-4} kPa at 25 °C

Method OECD TG 104 Vapour Pressure.
Remarks A vapour pressure balance was used to make the measurements.
Test Facility Harlan (2009a)

Water Solubility Miscible in water at 20 °C

Method In house method. OECD TG 105 was not used for this test substance due to its miscibility in water.
Remarks The test substance was mixed with water at concentrations of 5.11, 49.9 and 93.7%. The mixtures were shaken and then equilibrated at 20°C for 1 hour prior to visually examining the solubility. The pH for each solution was measured to be 9.2 – 9.5. All the solutions were uniform, clear and free from un-dissolved matter or separated phases. The 49.9% solution was viscous and the 93.7% solution was extremely viscous.

The notified chemical is pH sensitive. Based on the observation from the partition coefficient test (below), the notified chemical may degrade to form alkanolamine and carbon dioxide at the low concentration of 5.11%. The dissolved CO_2 is expected to form carbonate and bicarbonate in the solutions. Therefore, it is expected that low concentration solutions are complex mixtures and not the notified chemical as a whole.
Test Facility Harlan (2010a)

Partition Coefficient (n-octanol/water) log Pow = -1.78 at 22.5 ± 0.5°C

Method OECD TG 107 Partition Coefficient (n-octanol/water).
Remarks Shake Flask Method. The notified chemical was unable to be detected by high performance liquid chromatography with mass spectroscopy (HPLC-MS) during the determination of the partition coefficient. The notified chemical was concluded to degrade to the original reactants (alkanolamine and carbon dioxide) when it was diluted for the determination of the partition coefficient, based on the study author's

interpretation. Only alkanolamine was monitored during the test as carbon dioxide is a gas and was not detected. Therefore, the Pow value attained more likely reflects the Pow of the alkanolamine rather than the notified chemical. This is supported by the estimated value of log Pow = -1.61 for the alkanilamine, using KOCWIN, v.1.68 (US Environmental Protection Agency, 2011).

However, the notified chemical is a salt and would preferentially partition to the aqueous phase.

Test Facility Harlan (2009b)

Adsorption/Desorption – screening test log K_{oc} = -0.85

Method Estimated using KOCWIN, v. 2.00 (US Environmental Protection Agency, 2011)

Remarks The HPLC estimation method is not applicable for the notified chemical because it is an organic acid. Furthermore, the main degradation product, alkanolamine, was expected to interact with the HPLC column stationary phase by methods other than partitioning. The notifier provided an estimated value of log K_{oc} = -2.38 for the notified chemical. However, the attached estimation reports indicated that this value was for log P_{ow} rather than log K_{oc}.

Therefore, the adsorption coefficient was estimated by DSEWPaC based on the molecular connectivity index (MCI) and a series of statistically derived fragment contribution factors. The estimated value of log K_{oc} = -0.85 for the notified chemical has been used in this assessment. The adsorption coefficient was estimated to be log K_{oc} = 0.067 for the alkanolamine.

Test Facility Harlan (2010a)

Dissociation Constant pKa = 5.31 ± 0.41

Method Estimated using ACD/pKa, version 8.03, Advanced Chemistry Development, Inc.

Remarks No experimental testing was available since the notified chemical degrades in the acidic media. The dissociation constant (pKa) for the notified chemical was estimated to be 5.31 using the specialized predictive software.

The dissociation constant for the major degradation product, alkanolamine, was concluded to have a pKa value of 9.65 based on the average values from literature references.

Test Facility Harlan (2010a)

Flash Point No flash point below decomposition temperature

Method EC Council Regulation No 440/2008 A.9 Flash Point.

Remarks Measured using a closed cup.

Frothing indicative of decomposition was observed from ~104 °C.

Test Facility Harlan (2009a)

Autoignition Temperature > 400 °C

Method EC Council Regulation No 440/2008 A.15 Auto-Ignition Temperature (Liquids and Gases).

Remarks No signs of auto-ignition were observed at temperatures up to 400 °C. Grey fumes were emitted from 150 °C and above.

Test Facility Harlan (2009a)

Explosive Properties Not expected to be explosive

Method EC Council Regulation No 440/2008 A.14 Explosive Properties.

Remarks Test not conducted. The notified chemical does not contain functional groups which are

associated with explosive properties.
Test Facility Harlan (2009a)

Oxidizing Properties Not expected to be oxidising

Method EC Council Regulation No 440/2008 A.21 Oxidizing Properties (Liquids).
Remarks Test not conducted. The notified chemical does not contain functional groups that are expected to act as oxidizing agents.-
Test Facility Harlan (2009a)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Irritation – skin (in vitro)

TEST SUBSTANCE: Notified chemical

METHOD: Similar to OECD TG 439 *In Vitro* Skin Irritation: Reconstructed Human *Epidermis* Test Method
EpiSkin™ Reconstituted Human Epidermis Model.

Vehicle: None

Remarks - Method: The test substance (10 µL) was applied to the tissues in triplicate. Following 15 minute exposure periods, the tissues were rinsed and then incubated at 37 °C for approximately 42 hours.

Following treatment with MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide; 0.3mg/mL], the tissues were incubated at 37 °C for 3 hours.

Positive (sodium dodecyl sulphate; 5%) and negative (phosphate buffered saline) controls were run in parallel with the test substance.
The optical densities were determined at 540 nm.

RESULTS

Test Material	*Mean OD_{540} of triplicate tissues*	*± SD of OD_{540}*	*Relative mean viability (%)*	*± SD of relative mean viability (%)*
Negative Control	0.731	0.011	100*	1.5
Positive Control	0.031	0.007	4.2	0.9
Test Substance	0.741	0.030	101.4	4.0

OD = optical density; SD = standard deviation
*The mean viability of the negative control tissues is set as 100%.

Remarks - Results: The test substance was found to directly reduce MTT. Therefore, an additional procedure using water-killed tissues was performed to correct for direct reduction of MTT by the test substance that may remain absorbed to the cells after rinsing. Water-killed tissues possess no metabolic activity but absorb and bind the test substance like viable tissues. The results obtained with the water-killed tissues did not show any interference due to direct reduction of MTT, therefore no correction to the results was considered necessary.

The relative mean viability of the test substance treated tissues was 101.4% after a 15-minute exposure period.

The positive and negative controls gave satisfactory results, confirming the validity of the test system.

CONCLUSION: The notified chemical was non-irritating to the skin under the conditions of the test.

TEST FACILITY: Harlan (2010b)

B.2. Irritation – skin (in vitro)

TEST SUBSTANCE: Notified Chemical

METHOD: OECD TG 431 In vitro Skin Corrosion - Human Skin Model Test
EpiSkin™ Reconstituted Human Epidermis Model

Vehicle: None

Remarks - Method: The positive control used was glacial acetic acid and the negative control

was 0.9% w/v sodium chloride. Cell viability was measured by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay.

RESULTS

Test material	*Exposure Time*	*Mean OD_{540} of two tissues*[1]	*Relative mean Viability (%)*
Negative control	4 h	0.117	100[2]
Test substance	3 min	0.141	120.5
Test substance	1 h	0.144	123.1
Test substance	4 h	0.114	97.4
Positive control	4 h	0.008	6.8

OD = optical density
[1]Corrected for direct reduction of MTT by test substance
[2]The mean viability of the negative control tissues is set as 100%.

Remarks - Results

The test substance was found to directly reduce MTT. Therefore, an additional procedure using water-killed tissues was performed to correct for direct reduction of MTT by the test substance that may remain absorbed to the cells after rinsing. Water-killed tissues possess no metabolic activity but absorb and bind the test substance like viable tissues.

If direct MTT reduction by the test substance is greater than 30% of the negative control the assay results would not be considered viable. After 60 minutes the direct reduction was borderline at 30.8%. However, acceptable reduction was noted at 3 minutes (17.9%) and 4 h (25.6%). Given the test substance was clearly non-corrosive after a 4 h exposure the study authors considered the results were reliable.

The positive and negative controls gave satisfactory results, confirming the validity of the test system.

CONCLUSION

The notified chemical was non-corrosive to the skin under the conditions of the test.

TEST FACILITY

Harlan (2010c)

B.3. Irritation – skin

TEST SUBSTANCE

Notified chemical

METHOD

OECD TG 404 Acute Dermal Irritation/Corrosion.
EC Council Regulation No 440/2008 B.4 Acute Toxicity (Skin Irritation)

Species/Strain: Rabbit/New Zealand White
Number of Animals: 3 males
Vehicle: None
Observation Period: 72 hours
Type of Dressing: Semi-occlusive
Remarks - Method: No significant protocol deviations.

The pH of the test substance (as supplied) was 9.7.

A single rabbit was initially treated and then the additional rabbits were treated with the test substance in a similar fashion.

RESULTS

Lesion	*Mean Score* Animal No.*			*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3			

Erythema/Eschar	0	0	0	0	< 24 hours	0
Oedema	0	0	0	0	-	0

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

Remarks - Results: Very slight erythema was noted in one male 1 hour after patch removal, however, this had reversed by the 24 hourr observation.

CONCLUSION: The notified chemical is slightly irritating to the skin.

TEST FACILITY: Harlan (2010d)

B.4. Irritation – eye (in vitro)

TEST SUBSTANCE: Notified chemical

METHOD: Determination of Ocular Irritation Potential Using Reconstructed Human Corneal Epithelium Model

Remarks - Method: The test substance (30 µL) was applied to the tissues in triplicate. Following 10 minute exposure periods, the tissues (2/group, with the others being retained for histopathology if necessary) were rinsed and then treated with MTT (1 mL) [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide; 0.5 mg/mL; incubation period of 3 hours at 37 °C]. Following extraction, the optical densities were determined at 540 nm. Positive (sodium dodecyl sulphate; 1%) and negative controls were run in parallel with the test substance.
The test substance was considered by the study authors to be an irritant if the relative mean tissue viability was < 60%.

RESULTS

Test material	*Mean OD_{540} of duplicate tissues*	*Relative mean viability (%)*
Negative control	0.981	100*
Test substance	0.358	36.5
Positive control	0.783	79.8

OD = optical density
*The mean viability of the negative control tissues is set as 100%.

Remarks - Results: The test substance was found to directly reduce MTT. Therefore, an additional procedure using freeze-killed tissues was performed to correct for direct reduction of MTT by the test substance that may remain absorbed to the cells after rinsing. Freeze-killed tissues possess no metabolic activity but absorb and bind the test substance like viable tissues. The results obtained with the water-killed tissues did not show any interference due to direct reduction of MTT, therefore no correction to the results was considered necessary.

The relative mean viability of the test substance treated tissues after a 10-minute exposure period was 79.8%.

The positive and negative controls gave satisfactory results, confirming the validity of the test system.

CONCLUSION: The notified chemical was considered to be non-irritating to the eye under the conditions of the test.

TEST FACILITY: Harlan (2010e)

B.5. Irritation – eye

TEST SUBSTANCE: Notified chemical

METHOD: OECD TG 405 Acute Eye Irritation/Corrosion.
EC Council Regulation No 440/2008 B.5 Acute Toxicity (Eye Irritation)

Species/Strain: Rabbit/New Zealand White.
Number of Animals: 2 males
Observation Period: 7 days
Remarks – Method: No significant protocol deviations.

The pH of the test substance (as supplied) was 9.7.

A single rabbit was initially treated. Prior (1-2 minutes) to instillation of the test substance into the eye of second rabbit, a drop of local anaesthetic (tetracaine hydrochloride, 0.5%) was instilled into both eyes.

RESULTS

Lesion	*Mean Score* Animal No.*		*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2			
Conjunctiva: redness	1.7	1.7	2	< 7 days	0
Conjunctiva: chemosis	1	1	2	< 72 hours	0
Conjunctiva: discharge	1.7	1.3	3	< 7 days	0
Corneal opacity	0	0	0	-	0
Iridial inflammation	0.7	0.7	1	< 72 hours	0

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

Remarks - Results: Iridial inflammation was noted in both animals up to and including the 48 hour observation after treatment. Moderate conjuctival irritation was also noted in both animals up to 48 hours after treatment, however, this had reduced to minimal irritation by the 72 hour observation. No corneal opacity was noted. All effects were reversible within 7 days.

CONCLUSION: The notified chemical is slightly irritating to the eye.

TEST FACILITY: Harlan (2010f)

B.6. Skin sensitisation

TEST SUBSTANCE: Notified chemical

METHOD: OECD TG 406 Skin Sensitisation – Buehler Test
EC Directive (EC) No 440/2008 B.6 Skin Sensitisation – Buehler Test

Species/Strain: Guinea pig/Dunkin Hartley, Hsd Poc:DH
PRELIMINARY STUDY: Maximum Non-irritating Concentration:
topical: 25%

MAIN STUDY
Number of Animals: Test Group: 20 Females Control Group: 10 Females
INDUCTION PHASE: Induction Concentration:
topical: 50%
Signs of Irritation: Discrete or patchy erythema was noted in 3/20 animals after the first induction phase (test day 1), with desquamation and/or crusts present in an additional 8/20 animals. Discrete or patchy erythema was noted in 15/20 animals and moderate or confluent erythema was noted in 1/20 animals after the second induction phase (day 8), with desquamation and/or crusts present in 19/20 animals. Discrete or patchy erythema was noted in all animals after the third induction phase (day 15).

CHALLENGE PHASE
1st challenge: topical: 10%
Remarks - Method: No significant protocol deviations.

The vehicle was water. The challenge concentration (10%) was selected based on the observation of slight irritation in 2/3 animals in the preliminary study when treated with the test substance at 25% concentration.

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after: 1st challenge*	
		30 h	*54 h*
Test Group	10%	0/20	0/20
Control Group	10%	0/10	0/10

Remarks - Results: No signs of skin reactions were noted in either the control group or test group following challenge.

CONCLUSION: There was no evidence of reactions indicative of skin sensitisation to the notified chemical under the conditions of the test.

TEST FACILITY: Harlan (2011)

B.7. Genotoxicity – bacteria

TEST SUBSTANCE: Notified chemical

METHOD: OECD TG 471 Bacterial Reverse Mutation Test.
EC Directive 2000/32/EC B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria.
Plate incorporation procedure

Species/Strain: *S. typhimurium*: TA1535, TA1537, TA98, TA100
E. coli: WP2uvrA$^-$

Metabolic Activation System: S9 fraction from phenobarbitone/β-naphthoflavone induced rat liver

Concentration Range in Main Test: a) With metabolic activation: 0 - 5000 µg/plate
b) Without metabolic activation: 0 - 5000 µg/plate

Vehicle: Distilled water

Remarks - Method: No significant protocol deviations.

A preliminary study was conducted in the TA100 and WP2uvrA$^-$ strains in the presence and absence of metabolic activation between 0-5000 µg/plate.

Vehicle and positive controls (N-ethyl-N'-nitro-Nnitrosoguanidine for WP2uvrA$^-$, TA100 and TA1535, 9-Aminoacridine for TA 1537, and 4-Nitroquinoline-1-oxide for TA98) were used in parallel with the test substance.

The pH of the test substance formulations was determined in distilled water (ranged from 9.1 to 9.4 for 50 to 5000 µg/plate, respectively) and following buffering using 0.2 M phosphate buffer and nutrient broth (ranged from 7.6 to 9.3 for 50 to 5000 µg/plate, respectively).

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				

Test 1	> 5000	> 5000	> 5000	Negative
Test 2		> 5000	> 5000	Negative
Present				
Test 1	> 5000	> 5000	> 5000	Negative
Test 2		> 5000	> 5000	Negative

Remarks - Results: No significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains up to and including the maximum dose, either with or without metabolic activation.

The positive controls gave satisfactory responses, confirming the validity of the test system.

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

TEST FACILITY: Harlan (2010g)

B.8. Genotoxicity – in vitro

TEST SUBSTANCE: Notified chemical

METHOD: OECD TG 473 In vitro Mammalian Chromosome Aberration Test.
EC Directive 2000/32/EC B.10 Mutagenicity - In vitro Mammalian Chromosome Aberration Test.

Cell Type/Cell Line: human lymphocytes
Metabolic Activation System: S9 fraction from phenobarbitone/β-naphthoflavone induced rat liver
Vehicle: HEPES buffer (MEM)
Remarks - Method: No significant protocol deviations.

A preliminary study was conducted (4 hour exposure, with and without activation and 24 hour exposure without activation) at concentrations 6.49-1661.7 µg/mL.

Vehicle and positive controls (mitomycin C and cyclophosphamine) were run in parallel with the test substance.

The pH of the test substance formulations was determined and ranged from 7.35 to 8.03 for 6.50 to 1661.7 µg/mL, respectively.

Metabolic Activation	*Test Substance Concentration (µg/mL)*	*Exposure Period*	*Harvest Time*
Absent			
Test 1	0*, 51.93, 103.86, 207.71, 415.43*, 830.85*, 1661.7*	4 hours	24 hours
Test 2	0*, 51.93, 103.86, 207.71*, 415.43*, 830.85*, 1246.28, 1661.7	24 hours	24 hours
Present			
Test 1	0*, 51.93, 103.86, 207.71, 415.43*, 830.85*, 1661.7*	4 hours	24 hours
Test 2	0*, 51.93, 103.86, 207.71, 415.43*, 830.85*, 1661.7*	4 hours	24 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	> 1661.7	> 1661.7	> 1661.7	Negative
Test 2	≥ 1661.7	≥ 830.85	> 1661.7	Negative
Present				
Test 1	> 1661.7	> 1661.7	> 1661.7	Negative

Test 2	-	> 1661.7	> 1661.7	Negative

Remarks - Results	There were no statistically significant increases in the frequencies of cells with chromosomal aberrations at any tested concentration. The positive controls demonstrated a positive response, confirming the validity of the test system.
CONCLUSION	The notified chemical was not clastogenic to human lymphocytes treated in vitro under the conditions of the test.
TEST FACILITY	Harlan (2009c)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready biodegradability

TEST SUBSTANCE: Notified chemical

METHOD: OECD TG 301 D Ready Biodegradability: Closed Bottle Test.

Inoculum	Domestic sewage sludge micro-organisms
Exposure Period	28 days
Auxiliary Solvent	None
Analytical Monitoring	Dissolved oxygen meter, BOD probe and spectrophotometer
Remarks - Method	No significant protocol deviations. The test substance was dissolved directly in the culture media. The microorganisms were exposed to the medium in sealed vessels in the dark at around 21 °C. The dissolved oxygen concentration for each test medium was determined, in duplicate, on day 3, 5, 7, 11, 14, 21 and 28. As the test substance contains nitrogen, the observed oxygen consumption was corrected for the amount of oxygen used to oxidise ammonium to nitrite and nitrate.

RESULTS

Test substance		*Sodium benzoate*	
Day	*% Degradation*	*Day*	*% Degradation*
7	69	7	66
14	64	14	65
21	74	21	65
28	101	28	68

Remarks - Results

The oxygen depletion of the control did not exceed 1.5 mg O_2/L after 28 days. The residual oxygen concentration in the test bottles remained at 2.35 mg O_2/L or above for all the test vessels. The difference between the extremes of replicate oxygen depletion values at the end of the test was less than 20%. Therefore, all validation criteria were satisfied.

Based on the BOD determination, the test substance attained 101% degradation over 28 days and satisfied the 10-day window. The degradation value of greater than 100% was considered to be due to normal biological variation. The notified chemical is considered to be readily biodegradable under the Australian regulations.

Furthermore, based on the observation from the partition coefficient test (above), the notified chemical is expected to degrade under the ambient environment conditions to form CO_2 and alkanolamine. Alkanolamine attained 92% degradation (CO_2 production) over 28 days in a modified Strum test (Verschueren K, 1996). Therefore, the notified chemical can be considered to completely mineralise under environmental conditions.

Nitrate and nitrite analysis of the test solutions on day 28 confirmed that no significant oxygen consumption as a result of nitrification occurred during the test.

The degradability was 66% over 14 days and 89% after 28 in the toxicity control, indicating that the test material was not toxic to the sewage treatment micro-organisms.

CONCLUSION: The notified chemical is readily biodegradable

TEST FACILITY SafePharm (2008)

C.2. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE Notified chemical

METHOD OECD TG 203 Fish, Acute Toxicity Test – Flow through

Species	Rainbow trout (*Oncorhynchus mykiss*)
Exposure Period	96 hours
Auxiliary Solvent	None
Water Hardness	140 mg $CaCO_3$/L
Analytical Monitoring	Total organic carbon analysis (TOC)
Remarks – Method	No significant protocol deviations.

The stock solutions were prepared by directly dissolving the test substance in dechlorinated tap water. The pH of the stock solutions and the diluents used in the test was adjusted to approximately 7.5 as the test substance is pH sensitive. The stock solutions were freshly prepared daily prior to dosing by dynamic, continuous flow apparatus to give the test concentrations. The pH of the test media was measured to be 7.7-7.9.

In the range-finding test, three fish were exposed to the test solutions at nominal concentrations of 10 and 100 mg/L with one control run in parallel.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*3 h*	*24 h*	*48 h*	*72 h*	*96 h*
0	-	7	0	0	0	0	0
100	63-83*	14	0	0	0	0	0

* Based on the results of TOC analysis

LC50	> 100 mg/L at 96 hours.
NOEC	100 mg/L at 96 hours.
Remarks – Results	No analytical method could be identified for analysis of the test substance as it was anticipated to rapidly degrade to the original reactants. The test preparations were analysed for TOC only.

TOC analysis of the test preparations at 0, 24, 48, 72 and 96 hours indicated the measured concentrations for the test substance were within the range of 63-83 mg /L. The measured value is lower than anticipated, which was considered to result from the degradation of test substance.

Due to the rapid degradation of the test substance, the test fish would have been exposed to a mixture of products and not to the test substance as a whole. As the toxicity may be attributed to the mixture of degradation products and test substance, it was considered justifiable to base the results on nominal concentrations only.

CONCLUSION The notified chemical is not harmful to fish

TEST FACILITY Harlan (2010h)

C.2.2. Acute toxicity to aquatic invertebrates

TEST SUBSTANCE Notified chemical

METHOD OECD TG 202 *Daphnia* sp. Acute Immobilisation Test – Flow through

Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	None
Water Hardness	250 mg $CaCO_3$/L
Analytical Monitoring	Total organic carbon analysis (TOC)
Remarks - Method	No significant protocol deviations.

The stock solutions were prepared by directly dissolving the test substance in reconstituted water. The pH of the stock solutions and the diluents used in the test was adjusted to approximately 7.5 as the test substance is pH sensitive. The stock solutions were freshly prepared daily prior to dosing by dynamic, continuous flow apparatus to give the test concentrations. The pH of the test media was measured to be 7.5-7.7.

In the range-finding test, two groups of daphnids (10 per group) were exposed to the test solutions at a nominal concentration of 0.05, 0.5, 5.0 and 50 mg/L with one control run in parallel.

RESULTS

Concentration mg/L		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual**		*24 h*	*48 h*
0	N/A	10	0	0
5.0	5.3-5.4	20	0	0
9.0	8.3-9.1	20	0	4
16	16-19	20	1	3
28	28-39	20	1	6
50	44-46	20	3	16

* Based on the results of TOC analysis

LC50	32 mg/L at 48 hours (95% confidence limits of 24-48 mg/L)
NOEC	5.0 mg/L at 48 hours
Remarks - Results	No analytical method could be identified for analysis of the test substance as it was anticipated to rapidly degrade to the original reactants. The test preparations were analysed for TOC only.

TOC analysis of the test preparations at 0 and 48 hours indicated that the measured concentrations were 88-139% of the nominal concentrations for the test substance. Therefore, it was considered justifiable to base the results on nominal concentrations only.

Due to the rapid degradation of the test substance, the test daphnids would have been exposed to mixture products and not to the test substance as a whole. Hence, the toxicity may be attributed the mixture of the degradation products and the test substance.

CONCLUSION The notified chemical is harmful to aquatic invertebrates

TEST FACILITY Harlan (2010i)

C.2.3. Algal growth inhibition test

TEST SUBSTANCE Notified chemical

METHOD OECD TG 201 Alga, Growth Inhibition Test.

Species *Desmodesmus subspicatus*

Exposure Period	72 hours
Concentration Range	Nominal: Control, 6.25, 12.5, 25, 50 and 100 mg/L Actual: N/A, 6.31, 11.62, 23, 48 and 95 mg/L (based on Total Organic Carbon (TOC) content)
Auxiliary Solvent	None
Water Hardness	3 mg $CaCO_3$/L
Analytical Monitoring	TOC Coulter Multisizer Particle Counter
Remarks - Method	No significant protocol deviations. The stock solutions were prepared by directly dissolving the test substance in culture media. The pH of the stock solutions and the diluents used in the test was adjusted to approximately 7.5 as the test substance is pH sensitive. Growth inhibition was observed at concentrations of 1.0, 10 and 100 mg/L in the range-finding test. Based on the results of a preliminary range-finding test, two initial tests were conducted at concentrations of 0.10, 0.32, 1.0, 3.2 and 10 mg/L. The results of the initial tests indicated that no inhibition of growth at any of the concentrations applied. Therefore, the inhibition observed during the range-finding test was considered to be due to other unknown effects rather than from the chemical itself.

RESULTS

Biomass		*Growth*	
E_bC50 mg/L at 72 h	*NOE_bC mg/L at 72*	*E_rC50 mg/L at 72 h*	*NOE_rC mg/L at 72*
11	6.25	39	6.25
(95% confidence limits, 10-13 mg/L)		(Not determined)	

Remarks - Results	No analytical method could be identified for analysis of the test substance as it was anticipated to rapidly degrade to the original reactants. The test preparations were analysed for TOC only. TOC analysis of the test preparations at 0 and 72 hours indicated that the measured concentrations were 88-101% of the nominal concentrations for the test substance. Therefore, the test results were based on nominal concentrations. Due to the rapid degradation of the test substance, the test algae would have been exposed to a mixture of products and not to the test substance as a whole. Hence, the toxicity may be attributed the mixture of the degradation products and the test substance.

CONCLUSION The notified chemical is harmful to algae

TEST FACILITY Harlan (2010j)

BIBLIOGRAPHY

IUCLID (2008) [Analogue chemical]: European Commission, Joint Research Centre, Institute for Health and Consumer Protection, European Chemicals Bureau. Luxembourg, Belgium.

Harlan (2009a) Notified Chemical: Determination of Hazardous Physico-Chemical Properties (Study No. 1271/0036, April, 2009). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2009b) Notified Chemical: Determination of partition coefficient (Study No. 1271/0048, October, 2009). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2009c) Notified Chemical: Chromosome Aberration Test in Human Lymphocytes in vitro (Study No. 1271/0042, December, 2009). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010a) Notified Chemical: Determination of General Physico-Chemical Properties (Study No. 1271/0035, January, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010b) Notified Chemical: Determination of Skin Irritation Potential using the EpiskinTM Reconstituted Epidermis Model (Study No. 0334/0201, October, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010c) Notified Chemical: Determination of in vitro Skin Corrosion in the EpiskinTM Reconstituted Epidermis Model (Study No. 0334/0200, September, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010d) Notified Chemical: Acute dermal Irritation on the Rabbit (Study No. 0334/0206, October, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010e) Notified Chemical: Determination of Ocular Irritation Potential using the SkinEthic Reconstituted Human Corneal Epithelium Model (Study No. 0334/0202, October, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010f) Notified Chemical: Acute Eye Irritation in the Rabbit (Study No. 41003302), September, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010g) Notified Chemical: Reverse Mutation Assay (Ames) Test (Study No. 1271/0043), January, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010h) Notified Chemical: Acute toxicity to rainbow trout (*Oncorhynchus mykiss*) (Study No. 0334/0181, July, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2010i) Notified Chemical: Acute toxicity to *daphnia magna* (Study No. 0334/0182, July, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier)

Harlan (2010j) Notified Chemical: Algal growth inhibition test (Study No. 0334/0183, October, 2010). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

Harlan (2011) Notified Chemical: Contact Hypersensitivity in Albino Guinea Pigs, Buehler Test (Study No. D10513), March, 2011). Derbyshire, United Kingdom, Harlan Laboratories Ltd (Unpublished report submitted by the notifier).

NOHSC (2004) Approved Criteria for Classifying Hazardous Substances, 3rd edition [NOHSC:1008(2004)]. National Occupational Health and Safety Commission, Canberra, AusInfo.

NTC (National Transport Commission) 2007 Australian Code for the Transport of Dangerous Goods by Road and Rail (ADG code), 7th Edition, Commonwealth of Australia

SafePharm (2008) [Notified chemical]: Assessment of ready biodegradability; closed bottle test, (Study No. 1271/0047, July 2008) Derbyshire, UK, SafePharm Laboratories Limited, Castrol Industrial (Unpublished report submitted by the notifier)

SWA (2012) Code of Practice: Managing Risks of Hazardous Chemicals in the Workplace, Safe Work Australia, http://www.safeworkaustralia.gov.au/sites/swa/about/publications/pages/managing-risks-of-hazardous-chemicals-in-the-workplace.

United Nations (2009) Globally Harmonised System of Classification and Labelling of Chemicals (GHS), 3rd revised edition. United Nations Economic Commission for Europe (UN/ECE), <http://www.unece.org/trans/danger/publi/ghs/ghs_rev03/03files_e.html >.

US EPA (2011) Estimations Program Interface Suite™ for Microsoft® Windows, v 4.10. United States Environmental Protection Agency. Washington, DC, USA,http://www.epa.gov/oppt/exposure/pubs/episuite.htm, accessed 2013, May 16

Verschueren K (1996) Handbook of environmental data on organic chemicals, 3rd, New York, pp 930.