File No: LTD/1717 and LTD/1718

September 2014

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

PUBLIC REPORT

LTD/1717: Anthrazinesulfonic acid, 5,6,9,14,15,18-hexahydro-5,9,14,18-tetraoxo-

LTD/1718: Anthrazinedisulfonic acid, 5,6,9,14,15,18-hexahydro-5,9,14,18-tetraoxo-

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

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

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

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Director
NICNAS

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SUMMARY

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

ASSESSMENT REFERENCE	APPLICANT(S)	CHEMICAL OR TRADE NAME	HAZARDOUS CHEMICAL	INTRODUCTION VOLUME	USE
LTD/1717 LTD/1718	DIC Australia Pty Ltd	LTD/1717: Anthrazinesulfonic acid, 5,6,9,14,15,18-hexahydro-5,9,14,18-tetraoxo LTD/1718: Anthrazinedisulfonic acid, 5,6,9,14,15,18-hexahydro-5,9,14,18-tetraoxo-	ND*	LTD/1717: ≤ 1 tonne per annum LTD/1718: ≤ 1 tonne per annum	Components of inks and paints

*ND = not determined

CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification
Based on the available information, the notified chemicals are not recommended for classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals* (GHS), as adopted for industrial chemicals in Australia, or the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

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

When used in the proposed manner, the notified chemicals are 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 chemicals are not considered to pose an unreasonable risk to the environment.

Recommendations

CONTROL MEASURES

Occupational Health and Safety

- A person conducting a business or undertaking at a workplace should implement the following isolation and engineering controls to minimise occupational exposure to the notified chemicals during reformulation:
  - Enclosed, automated processes, where possible
  - Local exhaust 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 notified chemicals during reformulation:
  - Avoid contact with skin and eyes
  - Avoid inhalation

- 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 chemicals during reformulation:
  - Coveralls, impervious gloves and goggles

  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 chemicals 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 chemicals should be disposed of to landfill.

Emergency procedures

- Spills or accidental release of the notified chemicals 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 chemicals are listed on the Australian Inventory of Chemical Substances (AICS).

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

(1) Under Section 64(1) of the Act; if
  - the importation volume exceeds one tonne per annum for each notified chemical;

or

(2) Under Section 64(2) of the Act; if
  - the function or use of the chemicals has changed from components of inks and paints, or is likely to change significantly;
  - the amounts of chemicals being introduced have increased, or is likely to increase, significantly;
  - the chemicals have begun to be manufactured in Australia;
  - additional information has become available to the person as to an adverse effect of the chemicals 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 the notified chemicals and products containing the notified chemicals provided by the notifier were 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)
DIC Australia Pty Ltd (ABN: 12 000 079 550)
323 Chisholm Road
AUBURN NSW 2144

NOTIFICATION CATEGORY
LTD/1717: Limited-small volume: Chemical other than polymer (1 tonne or less per year) – Group Assessment.
LTD/1718: Limited-small volume: Chemical other than polymer (1 tonne or less per year) – Group Assessment.

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
No details are claimed exempt from publication.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
No variation to the schedule of data requirements is claimed.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
ISHL (Japan), 2013

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Sunfast® Blue (contains each of the notified chemicals at up to 3% concentration)

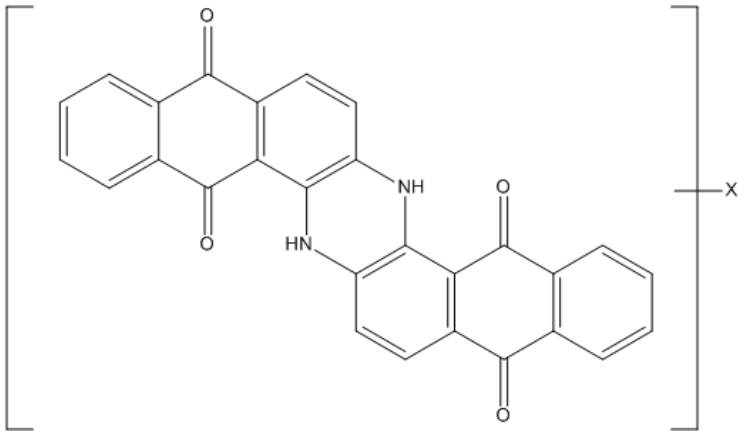
CAS NUMBER
LTD/1717: 28471-14-9
LTD/1718: 774119-48-1

CHEMICAL NAME
LTD/1717: Anthrazinesulfonic acid, 5,6,9,14,15,18-hexahydro-5,9,14,18-tetraoxo-
LTD/1718: Anthrazinedisulfonic acid, 5,6,9,14,15,18-hexahydro-5,9,14,18-tetraoxo-

OTHER NAME(S)
IB-SA (product containing 20-55% Mono-IBSA (LTD/1717) and 20-50% Di-IBSA (LTD/1718))
LTD/1717: Mono-IBSA, Monosulfonated Indanthrone Blue Sulfonic Acid
LTD/1718: Di-IBSA, Disulfonated Indanthrone Blue Sulfonic Acid

MOLECULAR FORMULA
LTD/1717: $C_{28}H_{14}N_2O_7S$
LTD/1718: $C_{28}H_{14}N_2O_{10}S_2$

STRUCTURAL FORMULA



LTD/1717: X = SO_3H
LTD/1718: X = $(SO_3H)_2$

MOLECULAR WEIGHT
LTD/1717: 522 Da
LTD/1718: 602 Da

ANALYTICAL DATA
Reference LC-MS and FTIR spectra were provided.

3. COMPOSITION
The notified chemicals are formed as part of an inseparable reaction mixture.

4. PHYSICAL AND CHEMICAL PROPERTIES
The following properties are for the reaction product mixture containing 20.4% Mono-IBSA (LTD/1717) and 45.1% Di-IBSA (LTD/1718).

APPEARANCE AT 20 °C AND 101.3 kPa: Dark blue powder

Property	Value	Data Source/Justification
Melting Point	Decomposes at > 250 °C	Measured*
Boiling Point	Not determined	Decomposes prior to melting*
Density	1,620 kg/m^3 at 20.8 ± 0.5 °C	Measured*
Vapour Pressure	2.8 × 10^{-7} kPa at 25 °C	Measured*
Water Solubility	4.48 × 10^{-2} g/L at 20 °C	Measured*
Hydrolysis as a Function of pH	$t_{1/2}$ > 1 year at 25 °C, pH 4-9	Measured*
Partition Coefficient (n-octanol/water)	log Pow = -0.334 at 22 °C	Measured*
Adsorption/Desorption	Not determined	The notified chemicals are expected to associate with soil and sediment based on their low water solubilities and anionic properties
Dissociation Constant	Not determined	The notified chemicals are organic acids and are expected to dissociate under environmental conditions (pH 4-9)
Particle Size	Inhalable fraction (< 100 μm): 41.6% Respirable fraction (< 10 μm): 1.11%	Measured*
Flammability	Not highly flammable	Measured*
Autoignition Temperature	365 °C	Measured*
Explosive Properties	Predicted negative	Based on thermal behaviour of the notified chemicals

Oxidising Properties	Predicted negative	Based on structure of the notified chemicals

* Test substance was the reaction product mixture containing 20.4% Mono-IBSA (LTD1717) and 45.1% Di-IBSA (LTD1718).

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

Reactivity
The notified chemicals are expected to be stable under normal conditions of use.

Physical hazard classification
Based on the submitted physico-chemical data depicted in the above table, the notified chemicals are 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 chemicals will be imported as a component (up to 3% each) of a formulated pigment product.

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

	Year	*1*	*2*	*3*	*4*	*5*
LTD/1717	*Tonnes*	0.1	0.15	0.25	0.4	1
LTD/1718	*Tonnes*	0.1	0.15	0.25	0.4	1

PORT OF ENTRY
Melbourne

IDENTITY OF MANUFACTURER/RECIPIENTS
Manufacturer: Sun Chemical Corporation (USA)
Recipient: DIC Australia Pty Ltd

TRANSPORTATION AND PACKAGING
The formulated pigment product containing the notified chemicals at up to 3% concentration (for each notified chemical) will be imported in 20 kg paper bags and transported by road or rail within Australia. The finished inks and paints containing the notified chemicals at up to 0.25% concentration (for each notified chemical) will be packaged to reflect the use of the final product i.e. inks will be packaged in containers/cartridges suitable for printing and paints will be packaged in canisters relevant to the application market.

USE
The notified chemicals will be used as a component (at up to 0.25% concentration for each notified chemical) of inks (used in commercial printers) (15-30% of total import volume) and automotive paints (70-85% of total import volume).

OPERATION DESCRIPTION
The notified chemicals will be imported as a component of a formulated pigment product (at up to 3% concentration for each notified chemical) for local reformulation into inks and automotive paints.

Reformulation
The imported pigment product containing the notified chemicals at up to 3% concentration (for each notified chemical) will be blended with other components to form finished ink/paint products through processes typically involving transferring between containers and the blending tank, mixing, QA testing, dispensing of finished products into suitable packages, and routine cleaning and maintenance. The finished products will contain the notified chemicals at up to 0.25% concentration (for each notified chemical).

End-Use
At a typical printing facility, the ink cartridge will be inserted into the printing machine or a pipe or hose will be connected to the containers holding the ink formulations and the ink containing the notified chemicals (at up to

0.25% concentration for each notified chemical) will be transferred to the printing machines fitted with exhaust ventilation via an automated and enclosed process. Any residual ink within printing equipment will be wiped clean using rags and solvents. These rags and dirty solvents are expected to be disposed of by the printing company through licensed waste disposal contractors.

At automotive manufacturing facilities, the application of paints containing the notified chemicals (at up to 0.25% concentration for each notified chemical) is expected to be largely automated and enclosed.

At automotive refinishing or repair sites, the paint containing the notified chemicals is expected be mainly applied by spray application in a dedicated spray booth. The level of ventilation present in the spray booth will vary between workshops. In smaller automotive refinish repair shops spray applications may occur outside of a spray booth.

6. HUMAN HEALTH IMPLICATIONS

6.1. Exposure Assessment

6.1.1. Occupational Exposure

Transport and Storage
Transport and storage workers may come into contact with the notified chemicals at up to 3% concentration (for each notified chemical) only in the event of an accidental rupture of containers.

Reformulation
Reformulation processes are expected to be largely enclosed and automated; however workers may be exposed (dermal and ocular) to the notified chemicals at up to 3% concentration (for each notified chemical) when transferring to the blending tank, during quality control testing and maintenance and cleaning tasks. Dermal and ocular exposure to workers should be mitigated through the use of personal protective equipment (PPE) including protective coveralls, impervious gloves and goggles. Inhalation exposure is expected to be low as the notified chemicals have a low vapour pressure at ambient temperatures. Inhalation exposure to dusts of the notified chemicals is also expected to be limited given the low concentration of the notified chemicals in the pigment product. Inhalation exposure to the notified chemicals should be further minimised through the use of local exhaust ventilation and enclosed processes.

End-use
Printer operators are not expected to be exposed to ink containing the notified chemicals at up to 0.25% concentration (for each notified chemical), as the process is expected to be mainly automated and enclosed. However, dermal exposure is possible to the notified chemicals during connection and disconnection of lines from containers of ink formulation to the printing machine and during printer maintenance. Exposure is expected to be limited by the use of PPE. Inhalation exposure may occur to aerosols of the notified chemicals during the operation of the printers. However, this is expected to be minimised by local exhaust ventilation employed in areas surrounding printing machines.

At automotive manufacturing facilities, exposure to the notified chemicals at up to 0.25% concentration (for each notified chemical) is likely to be low during the largely automated and isolated coating processes. Under normal conditions of operation, exposure to the notified chemicals would also be reduced by use of PPE.

At automotive refinishing or repair sites, dermal and ocular exposure to the notified chemicals at up to 0.25% concentration (for each notified chemical) may occur during spray application of the finished paints to automobile parts and when cleaning spray gun equipment. Exposure should be minimised where PPE consisting of coveralls, gloves and goggles are worn. The level of PPE will vary between workshops.

Due to the formation of aerosols, inhalation exposure is also likely during spray application, particularly where the level of ventilation within the spray booth is insufficient, application occurs outside of a spray booth and/or workers do not wear respirators.

Once the inks or paints are cured and dried, the notified chemicals will be bound within a solid matrix and will not be bioavailable.

6.1.2. Public Exposure

Ink and paint products containing the notified chemicals at up to 0.25% concentration (for each notified chemical) are only for use in industrial settings and will not be sold to the public. The public may come into contact with the inks or paints containing the notified chemicals after application to substrates. However, once the inks or paints are cured and dried, the notified chemicals will be bound within a solid matrix and will not be bioavailable.

6.2. Human Health Effects Assessment

The results from toxicological investigations conducted on a reaction product mixture containing 20.4% Mono-IBSA (LTD/1717) and 45.1% Di-IBSA (LTD/1718) are summarised in the following table. The remaining balance of the product mixture is reported to be comprised of 23.9% 6,15-dihydroanthrazine-5,9,14,18-tetrone (PB60) (CAS No. 81-77-6) and moisture. PB60 is the unsulfonated precursor to the notified chemicals and is expected to have a similar toxicological profile to the notified chemicals. Therefore, the results of the toxicological studies conducted on the reaction product mixture should provide an acceptable estimation of the toxicity of the notified chemicals. For full details of the studies, refer to Appendix B.

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	LD50 > 2000 mg/kg bw; low toxicity
Mutagenicity – bacterial reverse mutation	non mutagenic
Genotoxicity – in vitro chromosome aberration	non genotoxic

Toxicokinetic.

Based on the relatively high molecular weight (> 500 Da), low water solubility (4.48×10^{-2} g/L at 20 °C) and low partition coefficient (log Pow = -0.334 at 22 °C), absorption of the notified chemicals across biological membranes is expected to be limited. Furthermore the notified chemicals are strong acids. Ionised substances are generally considered not to cross biological membranes (ECB, 2003). The notified chemicals have a low vapour pressure but have a high proportion (41.6%) of particles in the inhalable size range (< 100 μm); hence inhalation exposure may only occur where aerosols are formed or when handling the powdered form of the notified chemicals. The notified chemicals contain only a small fraction (1.11%) of respirable particles (< 10 μm); hence the notified chemicals are not expected to reach the deep reaches of the lungs (alveolar air spaces), if inhaled, in significant quantities.

Acute toxicity.

A reaction product mixture containing 20.4% Mono-IBSA (LTD/1717), 45.1% Di-IBSA (LTD/1718) and PB60 was found to be of low acute oral toxicity in rats. There were no signs of systemic toxicity. Based on the results of this study, the notified chemicals are expected to be of low acute oral toxicity.

No acute dermal and inhalation toxicity data for the notified chemicals were submitted. The notified chemicals are expected to have limited potential for absorption; hence toxicity by the dermal and inhalation routes is not expected.

Irritation and sensitisation.

No irritation and sensitisation data for the notified chemicals were submitted. The notified chemicals contain structural alerts for skin (ketone) and eye irritation (sulfonic acid) (Hulzebos et al., 2005; Tsakovska et al., 2007). The potential for irritation may be limited by the relatively high molecular weight (> 500 Da).

The notified chemicals contain no structural alerts for sensitisation. Furthermore, the notified chemicals are expected to have limited potential for dermal absorption. Although it cannot be totally ruled out, the notified chemicals are expected to have limited potential for sensitisation.

Mutagenicity/Genotoxicity.

A reaction product mixture containing 20.4% Mono-IBSA (LTD/1717), 45.1% Di-IBSA (LTD/1718) and PB60 was found not mutagenic in a bacterial reverse mutation assay and not clastogenic to human lymphocytes in an *in vitro* chromosome aberration assay. Based on the results of these studies, the notified chemicals are not expected to be genotoxic.

Health hazard classification

Based on the available information, the notified chemicals are not recommended for classification according to the *Globally Harmonised System for the Classification and Labelling of Chemicals (GHS),* as adopted for

industrial chemicals in Australia, or the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

6.3. Human Health Risk Characterisation

6.3.1. Occupational Health and Safety

The notified chemicals are of low acute oral toxicity and are not expected to be genotoxic. Based on structural alerts the notified chemical may be irritating to the eye and skin, however this is expected to be limited given the relatively high molecular weight of the notified chemicals. Although it cannot be totally ruled out, the notified chemicals are expected to have limited potential for sensitisation. Toxicity from repeated exposure is not known, however, based on their physico-chemical properties the notified chemicals are likely to have limited potential for absorption.

During reformulation there is potential for dermal, ocular and inhalation exposure to the notified chemicals at up to 3% concentration, particularly when transferring the pigment product containing the notified chemicals to the blending tank. At these low concentrations, skin and eye irritation is not expected, however the potential risk of skin sensitisation, although limited, cannot be ruled out. The expected use of PPE should minimise exposure and any potential risk.

Inhalation exposure is expected to be low as the notified chemicals have a low vapour pressure at ambient temperatures. Inhalation exposure to dusts of the notified chemicals is also expected to be limited given the low concentration of the notified chemicals in the pigment product. Inhalation exposure to the notified chemicals should be further minimised through the use of local exhaust ventilation and enclosed processes during reformulation.

During end-use workers may be exposed to the notified chemicals at concentrations up to 0.25%. At these low end-use concentrations, the risk of adverse effects from use of the notified chemicals is not expected.

Given the low end-use concentration and stated controls in place to minimise exposure during reformulation, the risk to the health of workers is not considered unreasonable.

6.3.2. Public Health

The notified chemicals will be used in industrial settings only and will not be sold to the public. The public may come into contact with inks and paints containing the notified chemicals after application to substances. However, once the inks and paints are cured and dried, the notified chemicals will be bound within a coating matrix and will not be bioavailable. Therefore, when used in the proposed manner, the risk to public health is not considered to be unreasonable.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1. Environmental Exposure

RELEASE OF CHEMICAL AT SITE

The imported pigment containing the notified chemicals will be blended with other components in Australia to prepare printing inks and automotive paints. The blending activities are expected to occur 5-10 days per year at two to three industrial sites. The blending is expected to be largely automated and occur in enclosed systems. It is estimated by the notifier that up to 0.05% of the annual import volume of the notified chemicals, equivalent to 1 kg/year, may be released to the environment during these processes.

RELEASE OF CHEMICAL FROM USE

The notified chemicals are intended to be used as a component of inks for commercial/industrial printing (15-30% of total import volume) or as a component of paints for automotive painting (70-85%).

Inks containing the notified chemicals (up to 30% of the total import volume) are expected to be printed on paper. Once printing is complete, the notified chemicals are expected to be incorporated in an inert matrix and are not expected to be released from the printed paper. Ink cartridges are designed to prevent leakage and are not expected to be opened during transport, use, installation or replacement. Therefore, release of ink containing the

notified chemicals to the environment is not expected under normal conditions. Waste inks due to equipment cleaning or spillage is expected to be physically contained with absorbent material and disposed of to landfill.

Paints containing the notified chemicals (up to 85% of the total import volume) are expected to be used for automotive painting. During industrial spray application of formulated paints, the losses from overspray are expected to be captured by standard engineering controls and be disposed of to landfill. Once cured, the coatings containing the notified chemicals will form an inert paint matrix. The incorporated notified chemicals are not expected to be released to aquatic environment. Therefore, the release of the notified chemicals to aquatic environment is expected to be negligible.

RELEASE OF CHEMICAL FROM DISPOSAL

Printed waste paper containing the notified chemicals is expected to be disposed of to landfill or be subjected for paper recycling. During paper recycling processes, waste paper is repulped using a variety of chemical agents which, amongst other things, enhance detachment of ink from the fibres. The aqueous wastes from paper recycling are expected to be released to sewers and be directed to sewage treatment plants (STPs). Assuming half of the printed waste paper will be recycled, up to 15% (= 50% × 30%) of the notified chemicals are expected to be released to sewage systems.

Coated articles containing the notified chemicals are expected to be thermally decomposed during metal reclamation processes or disposed of to landfill along with the used articles.

Residual ink or paint products left in empty cartridges or empty containers will most likely be disposed of to landfill or be disposed of in compliance with local regulations.

7.1.2. Environmental Fate

The notified chemicals are expected to persist in the environment as they were determined to be hydrolytically stable and not readily biodegradable under environmental conditions. For the details of the environmental fate studies please refer to Appendix A and C.

Following their use as printing inks or automotive paints, the majority of the notified chemicals are expected to be cured into inert ink or paint matrices and share the fate of substrates to which they are applied. The majority of coated articles or printed paper is expected to be disposed of to landfill or subjected for metal reclamation or paper recycling. In landfill, the notified chemicals incorporated onto substrates' surface coatings are not expected to be bioavailable or bioaccumulative.

When used articles are subjected for metal reclamation, notified chemicals coated on these articles are expected to be thermally decomposed.

When printed waste paper is recycled, notified chemicals in printing ink may be released to sewers. During STP processes, the notified chemicals are expected to partially partition to sludge or sediment based on their low water solubilities and ionic properties. Sludge and sediment containing the notified chemicals are expected to be removed for disposal to landfill or applied to agricultural soil. Notified chemicals remaining in STP effluent are expected to be released to surface waters, where the notified chemicals are expected to disperse and eventually degrade.

The notified chemicals have potential to persist in the environment but are not expected to bioaccumulate due to their potential to ionise in the environment and the low measured n-octanol/water partition coefficient. The notified chemicals will eventually degrade in landfill, soil and water, or by thermal decomposition during metal reclamation processes, to form water and oxides of carbon, nitrogen and sulphur.

7.1.3. Predicted Environmental Concentration (PEC)

It was indicated by the notifier that up to 30% of total import volume of the notified chemicals will be used as inks and be printed on paper. Assuming 50% of used paper will be recycled, up to 15% (= 30% × 50%) of each of the notified chemicals is expected to be released to sewage systems as wastewater from paper recycling processes. A Predicted Environmental Concentration (PEC) for the worst case scenario has been calculated on the assumptions that the notified chemicals will be released nationwide to sewers over 260 days/year and there is no removal of the notified chemicals at STPs.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment

LTD/1717 LTD/1718

Total Annual Import/Manufactured Volume	1,000	1,000	kg/year
Proportion expected to be released to sewer	15%	15%	
Annual quantity of chemical released to sewer	150	150	kg/year
Days per year where release occurs	260	260	days/year
Daily chemical release:	0.58	0.58	kg/day
Water use	200	200	L/person/day
Population of Australia (Millions)	22.613	22.613	million
Removal within STP	0%	0%	
Daily effluent production:	4,523	4,523	ML
Dilution Factor - River	1.0	1.0	
Dilution Factor - Ocean	10.0	10.0	
PEC - River:	0.13	0.13	µg/L
PEC - Ocean:	0.013	0.013	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 chemicals in this volume are assumed to infiltrate and accumulate in the top 10 cm of soil (density 1500 kg/m^3). Using these assumptions, irrigation with a concentration of 0.13 µg/L may potentially result in a soil concentration of approximately 0.85 µg/kg for each notified chemical. Assuming accumulation of the notified chemicals in soil for 5 and 10 years under repeated irrigation, the concentration of each notified chemical in the applied soil in 5 and 10 years may be approximately 4.25 µg/kg and 8.5 µg/kg, respectively.

7.2. Environmental Effects Assessment

The result from ecotoxicological investigations conducted on a test substance reportedly containing 50% Mono-IBSA (LTD1717) and 50% Mono-IBSA (LTD1718) is summarised in the table below. Details of this study can be found in Appendix C.

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	LC50 (96 h) > 4.39 mg/L	May be toxic to fish

The notified chemicals are considered to be potentially toxic to fish on the acute basis as it has not been demonstrated that the median lethal concentration (LC50) is greater than 10 mg/L. However, this test was conducted at a limit concentration of 4.39 mg/L and no toxic symptoms or mortality were observed in control and test groups. The exact LC50 value was unable to be derived based on this result. Therefore, the notified chemicals are not formally classified under the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS, United Nations, 2009).

The exact LC50 value was unable to be derived based on the above result and there were no chronic ecotoxicity endpoints available. Therefore, the notified chemicals are not formally classified for their chronic hazard under the GHS.

7.2.1. Predicted No-Effect Concentration

The Predicted No-Effect Concentration (PNEC) was calculated using the fish toxicity endpoint (96 hours, LC50 > 4.39 mg/L) and a conservative assessment factor of 1000. An assessment factor of 1000 was used as the ecotoxicity endpoint for only one trophic level was available.

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
LC50 (Fish)	> 4.39	mg/L
Assessment Factor	1000	
PNEC:	> 4.39	µg/L

7.3. Environmental Risk Assessment

Risk Assessment	PEC µg/L	PNEC µg/L	Q
LTD/1717			
Q - River	0.13	> 4.39	**< 0.03**
Q - Ocean	0.013	> 4.39	**< 0.003**

LTD/1718			
Q - River	0.13	> 4.39	**< 0.03**
Q - Ocean	0.013	> 4.39	**< 0.003**

The risk quotients (Q = PEC/PNEC) for aquatic exposure have been calculated to be < 1. Although the notified chemicals have potential to be released into waterways, they are unlikely to pose a risk to the aquatic environment given that they are not expected to be released at ecotoxicologically significant concentrations. Therefore, on the basis of the PEC/PNEC ratio and the assessed use pattern, the notified chemicals are not considered to pose an unreasonable risk to the environment.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Melting Point Decompose at ~ 250 °C

Method OECD TG 102 Melting Point/Melting Range.
EC Council Regulation No 440/2008 A.1 Melting/Freezing Temperature.
Remarks Determined by differential scanning calorimetry.
Test Facility Harlan (2013)

Density 1,620 kg/m^3 at 20.8 ± 0.5 °C

Method OECD TG 109 Density of Liquids and Solids.
EC Council Regulation No 440/2008 A.3 Relative Density.
Remarks Determined using a gas comparison pycnometer.
Test Facility Harlan (2013)

Vapour Pressure < 2.8 × 10^{-7} kPa at 25 °C

Method OECD TG 104 Vapour Pressure.
EC Council Regulation No 440/2008 A.4 Vapour Pressure.
Remarks Determined using the vapour pressure balance method.
Test Facility Harlan (2012a)

Water Solubility 4.48 × 10^{-2} g/L at 20 °C

Method OECD TG 105 Water Solubility.
Remarks Flask Method. The test solutions (three replicates) were shaken at 30 °C for 94, 120 and 144 hours, respectively. The solutions were allowed to equilibrate for 24 hours at 20 °C. The concentrations of the test substance in each solution were determined by spectrophotometric method. The pH of the test solutions was determined to be 4.7, 4.8 and 4.9.
Test Facility Harlan (2013)

Hydrolysis as a Function of pH $t_{1/2}$ > 1 year at 25 °C

Method OECD TG 111 Hydrolysis as a Function of pH.

pH	*T (°C)*	*$t_{½}$ <years>*
4	25	> 1
7	25	> 1
9	25	> 1

Remarks At 50 °C, less than 10% hydrolysis was observed after incubation of the test substance for 5 days at pH 4, 7 and 9, equivalent to $t_{1/2}$ > 1 year at 25 °C. Therefore, the test substance was considered to be hydrolytically stable at the test conditions.
Test Facility Harlan (2013)

Partition Coefficient (n-octanol/water) log Pow = -0.334 at 22 °C

Method OECD TG 107 Partition Coefficient (n-octanol/water).
Remarks Flask Method. After partitioning, a rippled skin like layer was observed at the phase boundary which was darker blue than the colour of water and octanol phase. The recovery of the test substance was only 37.4 to 61.6%. Hence, the test substances may be surface active.

The test was performed with the test substances in their ionised forms as the test substances contains functionalities that are expected to dissociate at environmental conditions (pH 4-9). Therefore, the partition coefficient may not be accurately determined by this method. The result should be treated with caution.

Test Facility Harlan (2013)

Particle Size

Method OECD TG 110 Particle Size Distribution/Fibre Length and Diameter Distributions.

Range (μm)	*Mass (%)*
< 100	41.6
< 10	1.11
< 5.5	0.232

Remarks Determined using a 100 μm sieve in screening test and a Marple Miller Cascade Impactor in definitive test. Too few particles were of a size < 10 μm to allow accurate assessment of mass median aerodynamic diameter.
Test Facility Harlan (2013)

Flammability Not highly flammable

Method EC Council Regulation No 440/2008 A.10 Flammability (Solids).
Remarks Determined by measuring the burning rate of the test substance.
Test Facility Harlan (2012b)

Autoignition Temperature 365 °C

Method EC Council Regulation No 440/2008 A.16 Relative Self-Ignition Temperature for Solids.
Remarks The test substance was heated in a fine mesh stainless steel cube that is suspended in an oven.
Test Facility Harlan (2012b)

Explosive Properties Predicted negative

Method EC Council Regulation No 440/2008 A.14 Explosive Properties.
Remarks Predicted negative based on the absence of any sharp exotherms when heated up to 500 °C by differential scanning calorimetry.
Test Facility Harlan (2012b)

Oxidizing Properties Predicted negative

Method EC Council Regulation No 440/2008 A.17 Oxidizing Properties (Solids).
Remarks Predicted negative based on the chemical structure of the test substance.
Test Facility Harlan (2012b)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE	Reaction product mixture containing 20.4% Mono-IBSA (LTD1717), 45.1% Mono-IBSA (LTD1718) and 23.9% PB60
METHOD	OECD TG 420 Acute Oral Toxicity - Fixed Dose Method. EC Council Regulation No 440/2008 B.1 Acute Toxicity (Oral).
Species/Strain	Rat/Wistar
Vehicle	Arachis oil BP

RESULTS

Sighting Study

Dose mg/kg bw	*Number and Sex of Animals*	*Evident Toxicity*	*Mortality*
2000	1 female	No effects observed	None
300	1 female	No effects observed	None

Signs of Toxicity	No sign of systemic toxicity.
Effects in Organs	No abnormalities noted at necropsy.

Main Study

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
2000 mg/kg	4 females	2000	None

Signs of Toxicity	No sign of systemic toxicity.
Effects in Organs	No abnormalities noted at necropsy.

CONCLUSION	The test substance is of low toxicity via the oral route.
TEST FACILITY	Harlan (2012c)

B.2. Genotoxicity – bacteria

TEST SUBSTANCE	Reaction product mixture containing 20.4% Mono-IBSA (LTD1717), 45.1% Mono-IBSA (LTD1718) and 23.9% PB60
METHOD	OECD TG 471 Bacterial Reverse Mutation Test. EC Council Regulation No 440/2008 B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria. Plate incorporation procedure and pre incubation procedure
Species/Strain	*S. typhimurium*: TA1535, TA1537, TA98, TA100 *E. coli*: WP2uvrA
Metabolic Activation System	S9 mix from phenobarbitone/β-naphthoflavone induced rat livers
Concentration Range in Main Test	a) With metabolic activation: 50-5000 µg/plate b) Without metabolic activation: 50-5000 µg/plate
Vehicle	Distilled water
Remarks - Method	A preliminary toxicity test (0-5000 µg/plate) was performed against each tester strain to determine the toxicity of the test substance. In the mutation studies (using plate incorporation in range-finding test and pre-incubation in main test), aliquots of 0.4 mL of either test substance or negative control formulation or 0.1 mL of positive control formulation, was used at five concentrations up to 5000 µg/plate. The negative control was distilled water and positive controls were N-ethyl-N'-nitro-N-nitrosoguanidine, 9-aminoacridine, and 4-nitroquinoline-1-oxide in the absence of S9 mix and 2-aminoanthracene and benzo[a]pyrene in the

presence of S9 mix.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	> 5000	> 5000	≥ 500	Negative
Test 2		> 5000	≥ 500	Negative
Present				
Test 1	> 5000	> 5000	≥ 500	Negative
Test 2		> 5000	≥ 500	Negative

Remarks - Results

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

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

CONCLUSION

The test substance is not mutagenic to bacteria under the conditions of the test.

TEST FACILITY

Harlan (2012d)

B.3. Genotoxicity – in vitro

TEST SUBSTANCE

Reaction product mixture containing 20.4% Mono-IBSA (LTD1717), 45.1% Mono-IBSA (LTD1718) and 23.9% PB60

METHOD

OECD TG 473 In vitro Mammalian Chromosome Aberration Test.
EC Council Regulation No 440/2008 B.10 Mutagenicity – in vitro mammalian chromosome aberration test.

Species/Strain
Cell Type/Cell Line — Human lymphocytes
Metabolic Activation System — S9 mix from phenobarbitone/β-naphthoflavone induced rat livers
Vehicle — Eagle's minimal essential medium with HEPES buffer (MEM)
Remarks - Method — Doses up to 32 µg/mL were chosen in a dose-finding study (using short-time treatment method and continuous treatment method) on the basis that metaphase cells were present up to 31.25 µg/mL in both of the treatments in the absence of metabolic activation and up to 125 µg/mL in the short-time treatment in the presence of metabolic activation.

The negative control was MEM and positive controls were mitomycin C in the absence of S9 mix and cyclophosphamide in the presence of S9 mix.

Metabolic Activation	*Test Substance Concentration (µg/mL)*	*Exposure Period*	*Harvest Time*
Absent			
Test 1	2*, 4*, 8*, 16, 24, 32	4	24
Test 2	1, 2*, 4*, 8*, 16, 32	24	24
Present			
Test 1	1, 2*, 4*, 8*, 16*, 32	4	24
Test 2	1, 2, 4*, 8*, 16*, 32	4	24

*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	≥ 7.82	> 8	≥ 2	Negative
Test 2	≥ 62.5	> 8	≥ 1	Negative
Present				
Test 1	≥ 62.5	> 16	≥ 1	Negative
Test 2		> 16	≥ 4	Negative

Remarks - Results The test substance did not induce any statistically significant increases in the frequency of cells with aberrations in any of the exposure groups.

CONCLUSION The test substance is not clastogenic to human lymphocytes treated in vitro under the conditions of the test.

TEST FACILITY Harlan (2012e)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Environmental Fate

C.1.1. Ready biodegradability

TEST SUBSTANCE	Reaction product mixture containing 20.4% Mono-IBSA (LTD1717), 45.1% Mono-IBSA (LTD1718) and 23.9% PB60
METHOD	OECD TG 301 B Ready Biodegradability: CO_2 Evolution Test.
Inoculum	Activated sludge
Exposure Period	28 days
Auxiliary Solvent	None
Analytical Monitoring	TOC analyser
Remarks - Method	The test substance was dispersed directly into the test medium. Two replicates were prepared for each test. The tests were conducted in accordance with the test guideline. There was no significant deviation from the protocol was reported. Good Laboratory Practice (GLP) was followed.

RESULTS

Test substance		*Sodium benzoate*	
Day	*% Degradation*	*Day*	*% Degradation*
0	0	0	0
8	6	8	20
14	9	14	87
21	1	21	83
28	2	28	81
29	8	29	85

Remarks - Results	All validity criteria for the test were satisfied. The day 29 values were corrected to include any carry-over of CO_2 detected in the second CO_2 absorber vessels. The toxicity control attained 53% and 56% degradation after 28 days. Therefore, the test substance was not considered toxic to the sewage treatment microorganisms used in the test.
CONCLUSION	The test substance is not readily biodegradable.
TEST FACILITY	Harlan (2012f)

C.2. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE	Mixture containing 50% Mono-IBSA (LTD1717) and 50% Mono-IBSA (LTD1718)
METHOD	OECD TG 203 Fish, Acute Toxicity Test – Semi-static.
Species	Zebra fish (*Danio rerio*)
Exposure Period	96 hours
Auxiliary Solvent	None
Water Hardness	Not Reported
Analytical Monitoring	High Performance Liquid Chromatography (HPLC)
Remarks – Method	Fish were exposed in the test media under semi-static conditions. The test media were renewed every 24 hours. The fish were observed for toxic signs (e.g. discoloration, lethargy, slowly swimming, and loss of equilibrium, curve and haemorrhage) at 2, 24, 48, 72 and 96 hours after

initial exposure.

The test was conducted in accordance with the test guideline apart from the water hardness of the test media was not tested or reported. The Good Laboratory Practices (GLP) was followed.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*2 h*	*24 h*	*48 h*	*72 h*	*96 h*
Control	-	7	0	0	0	0	0
5	4.39	7	0	0	0	0	0

LC50 > 4.39 mg/L at 96 hours.

Remarks – Results In the preliminary test, no dead fish were observed at the nominal test concentrations of 5, 10, 20 and 40 mg/L. However, the solutions at the nominal concentrations 10, 20 and 40 mg/L were stratified after 24 hours settlement and tiny fine granules were visually observed.

Samples were taken in the upper layer from the 5 mg/L solution, the measured concentration of 24 hours solution was 95.4% of the 0 h solution. The test solution of 5 mg/L was considered acceptable for the following definitive limit test.

During the 96 hours exposure time period in the definitive test, no toxic symptoms and mortality were observed in the control and test groups. All validity criteria for the test were satisfied. However, as it has not been demonstrated that the LC50 is greater than 10 mg/L, the test substance may be toxic to fish.

CONCLUSION The test substance may be toxic to fish.

TEST FACILITY SCC (2013)

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