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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Polyquaternium-68

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 the Environment, Water, Heritage and the Arts.

For the purposes of subsection 78(1) of the Act, this Full Public Report may be inspected at our NICNAS office by appointment only at 334-336 Illawarra Road, Marrickville NSW 2204.

This Full 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

TABLE OF CONTENTS

FULL PUBLIC REPORT

Polyquaternium-68

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
BASF Australia Limited (ABN 62 008 437 867)
500 Princes Highway
Noble Park, VIC 3174

NOTIFICATION CATEGORY
Limited: Synthetic polymer with Mn ≥ 1000 Da.

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
Data items and details claimed exempt from publication: other names, structural formula, molecular formula, molecular weight, spectral data, purity, identity of impurities, import volume, customer identity, polymer constituents and residual monomers.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: density, vapour pressure, adsorption/desorption, dissociation constant, flash point, flammability limits and autoignition temperature.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None

NOTIFICATION IN OTHER COUNTRIES
Canada

2. IDENTITY OF CHEMICAL

CHEMICAL NAME
1H-Imidazolium, 1-ethenyl-3-methyl-, methyl sulfate (1:1), polymer with 1-ethenyl-1H-imidazole, 1-ethenyl-2-pyrrolidinone and 2-methyl-2-propenamide.

MARKETING NAME(S)
Luviquat Supreme (contains the notified polymer at a concentration of 18 - 21%)

OTHER NAME(S)
INCI Name: Polyquaternium-68
Copolymer of vinylpyrrolidinone, methacrylamide, vinylimidazole and quaternized vinylimidazole.

CAS NUMBER
827346-45-2

MOLECULAR WEIGHT
Mn > 10,000 Da

ANALYTICAL DATA
Reference NMR and GPC spectra were provided.

3. COMPOSITION

DEGREE OF PURITY > 98%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS

Hazardous impurities are present at concentrations below the requirements for classification.

NON HAZARDOUS IMPURITIES/RESIDUAL MONOMERS (> 1% by weight) None

ADDITIVES/ADJUVANTS None

LOSS OF MONOMERS, OTHER REACTANTS, ADDITIVES, IMPURITIES
None under normal conditions of use.

DEGRADATION PRODUCTS
No degradation, decomposition or depolymerisation of the notified polymer is expected to occur under normal conditions of use.

The MSDS indicates that thermal decomposition begins at 310°C.

4. PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE AT 20°C AND 101.3 kPa: Colourless to slightly yellow liquid with faint odour (for 18 - 21% aqueous solution)

Property	Value	Data Source/Justification
Melting Point/Freezing Point	Not determined	The notified polymer will be imported as a component of an aqueous solution.
Boiling Point	Not determined	The notified polymer will be imported as a component of an aqueous solution.
Density	1053 kg/m^3 at 20°C	MSDS (for the aqueous product containing the notified polymer at 18 - 21%).
Viscosity	3,000-20,000 mPa.s at 23°C	MSDS (for the aqueous product containing the notified polymer at 18 - 21%).
Vapour Pressure	< 1.3 × 10^{-9} kPa	Estimated based on the NAMW > 1,000 Da (US EPA, 2007).
Water Solubility	> 390 and < 500 g/L at 23°C, at both pH 2 and in demineralised water > 380 and < 480 g/L at 23°C, at both pH 7 and 9.	Visual method.
Hydrolysis as a Function of pH	Hydrolytically stable, pH 4 - 9	Measured.
Partition Coefficient (n-octanol/water)	log Pow < -4.9 at 20°C	Estimated from the solubilities in water and n-octanol.
Adsorption/Desorption	Not determined.	Given the cationic nature of the notified polymer, it is expected to associate with the soil matrix.
Dissociation Constant	Not determined	The notified polymer is expected to remain fully dissociated due to the quaternary imidazolium group.
Flash Point	Not determined	The notified polymer will be imported as a component of an aqueous solution.
Flammability	Not determined	Not expected to be flammable under normal conditions of use.
Autoignition Temperature	Not determined	Not expected to autoignite under normal conditions of use.
Explosive Properties	Not expected to be explosive	The structural formula contains no explosophores.

DISCUSSION OF PROPERTIES

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

Reactivity
Stable under normal conditions of use.

5. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified polymer will not be manufactured within Australia. The notified polymer will be imported as a component (18 - 21% in an aqueous solution) of the product Luviquat Supreme, in 120 L plastic (PE) open head drums.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	1-10	1-10	1-10	1-10	1-10

PORT OF ENTRY
MELBOURNE

IDENTITY OF MANUFACTURER/RECIPIENTS
BASF Australia Pty Ltd
500 Princes Highway
Noble Park, VIC 3174

TRANSPORTATION AND PACKAGING
The 120 L plastic (PE) open head drums containing the notified polymer (18 - 21%) will be transported by road throughout Australia. The finished products containing the notified polymer at concentration of 0.4 - 2.0% will be packaged in containers ranging from 100 to 250 mL.

USE
Styling polymer for hair mousses at concentrations of 0.4 - 2.0%.

Approximately 70% of the introduced notified polymer will be in products used in commercial outlets with the remaining 30% used by the public.

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

The imported product containing the notified polymer at 18 - 21% will undergo quality assurance tests prior to being reformulated. The imported product will be transferred using a sparge and pump into tanks and compounded into finished products, which contain the notified polymer at concentrations of 0.4 - 2.0%. Following further quality control testing the finished products containing the notified polymer will be pumped into the finished pack using automated lines.

The finished products will be used by hairdressers who will generally apply the products by hand.

6. HUMAN HEALTH IMPLICATIONS

6.1 Exposure assessment

6.1.1 Occupational exposure

NUMBER AND CATEGORY OF WORKERS

Category of Worker	*Number*	*Exposure Duration (hours/day)*	*Exposure Frequency (days/year)*
Transportation and warehousing	2-4	2	20
Laboratory/quality assurance	2-4	7	50
Plant operators – weighing and compounding	4-6	8	50
Plant operators – filling and packaging	2-4	2	20
Hairdressing salon workers	> 1000	1-2	200

EXPOSURE DETAILS

Transport and storage

Transport and warehouse workers will be exposed to the notified polymer only in the event of a spill due to an accident or leaking drum. Workers may wear protective overalls, hard hats, chemical resistant gloves and safety glasses.

Reformulation

At customer reformulation facilities, exposure to the notified polymer (at up to 21%) is possible during handling of the drums, cleaning and maintenance of the equipment. When handling the imported product (18 – 21% notified polymer) and reformulated products (0.4 – 2.0% notified polymer) dermal, and eye contact (due to splashing) are likely to be the main routes of exposure. Exposure is likely to be minimised by good personal hygiene practices (eg. washing hands after any contact, before breaks and meals, etc) and use of industrial standard PPE. Inhalation exposure is likely to be negligible due to the low vapour pressure of the notified polymer.

End use

Exposure of hairdressers to the notified polymer at concentrations of 0.4 – 2.0% is likely to occur during final application of the cosmetic products to their clients. The main route of exposure is expected to be dermal, although accidental ocular exposure is possible. PPE is not expected to be worn, however good hygiene practices may be in place.

6.1.2. Public exposure

The public is expected to be exposed to the notified polymer at concentrations of 0.4 – 2.0% during the use of hair styling products. The maximum dermal exposure to the product estimated using consumer exposure data (SCCP, 2006) was 10 g/day (5 g/use). The retention factor for hair styling products is assumed to be 0.1. Assuming a default consumer body weight of 60 kg (for females) and 10% dermal absorption (due to the high molecular weight) the exposure is estimated to be 0.029 mg/kg bw/day.

Since products containing the notified polymer are stored and used in a domestic environment, there is the possibility of accidental ingestion by a child.

6.2. Human health effects assessment

The results from toxicological investigations conducted on the Luviquat Supreme (containing 18 – 21% notified polymer in an aqueous solution) are summarised in the table below. Details of these studies can be found in Appendix B.

Endpoint	*Result and Assessment Conclusion*
Rat, acute oral toxicity	oral LD50 > 2000 mg/kg bw
Rabbit, skin irritation	slightly irritating
Rabbit, eye irritation	slightly irritating
Guinea pig, skin sensitisation – non-adjuvant test.*	no evidence of sensitisation
Mutagenicity – bacterial reverse mutation	non mutagenic
Genotoxicity – in vitro mammalian chromosome aberration test	non genotoxic

* Conducted using 75% Luviquat Supreme i.e. 13-16% notified polymer.

Toxicokinetics, metabolism and distribution.
The notified polymer is not expected to be absorbed across biological membranes, based on the high molecular weight (> 10,000 Da).

Acute toxicity.
No signs of toxicity were observed in rats dosed orally with Luviquat Supreme (18 – 21% notified polymer) at 2000 mg/kg bw. The LD50 of the notified polymer is therefore > 360 – 420 mg/kg bw, however it is not expected to be harmful via the oral route due to the expected low absorption.

Irritation and Sensitisation.
Based on a test conducted on rabbits with Luviquat Supreme (18 – 21% notified polymer) the notified polymer is considered to be at least slightly irritating to the skin and eye. Luviquat Supreme (notified polymer) was found to be a non-sensitiser in a Buehler test on guinea pigs. Based on this result, and the high molecular weight, the notified polymer is not likely to be a skin sensitiser.

Mutagenicity and carcinogenicity.
Luviquat Supreme (18 – 21% notified polymer) was found to be not mutagenic using a bacterial reverse mutation test, and not clastogenic to Chinese hamster V79 cells *in vitro*.

Health hazard classification
Based on the available data the notified polymer is not classified as hazardous under the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

6.3. Human health risk characterisation

6.3.1. Occupational health and safety
The highest occupational exposure to the notified polymer (at up to 21%) is expected to be to reformulation workers during handling of the drums, cleaning and maintenance of the equipment. Significant dermal exposure may also occur for hairdressers using the finished cosmetic products (0.4 – 2.0% notified polymer).

Local effects
The notified polymer itself is considered to be at least a slight skin and eye irritant and non-sensitising. The exposure is expected to be minimised by the reduced concentration (18 – 21%) and proposed use of personal protective equipment in the case of reformulation workers, and the lower concentrations (0.4 – 2.0%) and good hygiene practices in the case of hairdressers. Therefore the risk of irritant effects after exposure to the notified polymer is not considered to be unacceptable.

Systemic effects
The systemic effects of the notified polymer have not been tested. Oral exposure is expected to be low and is likely to be minimised further by good personal hygiene practices. The main route of exposure by workers is expected to be dermal, however the potential for systemic exposure is expected to be low given the high molecular weight (> 10,000 Da) of the notified polymer. Therefore the risk to workers from exposure to the notified polymer is not be considered unacceptable.

6.3.2. Public health
The public is expected to be exposed to the notified polymer at concentrations of 0.4 – 2.0% during the use of hair styling products. The exposure and hazard of the notified polymer to members of the public during use of the hair styling products are expected to be similar, or to a lesser extent to that experienced by hairdressers.

Any one off ingestion of the notified polymer is unlikely to pose a risk due to the expected low acute oral toxicity of the notified polymer at concentrations present in the finished cosmetic products.

Overall, the risk of the notified polymer to the health of the public is considered to be low.

7. ENVIRONMENTAL IMPLICATIONS

7.1. Environmental Exposure & Fate Assessment

7.1.1 Environmental Exposure

RELEASE OF CHEMICAL AT SITE

Release to the environment may occur in the unlikely event of an accident during transport or an accidental spill. The notified polymer will be transported to Australia by ship in 120 L plastic drums and will be transported by road to the importer's warehouse and then to the customer's formulation site.

During the formulation of the hair care products up to 1% per annum of the imported volume of notified polymer will be released into the environment as a result of residues in import containers, spills and equipment cleaning. Waste from container and equipment cleaning will be disposed to the sewer. Residues along with their empty containers will be disposed to landfill. Spills will also be disposed to landfill.

RELEASE OF CHEMICAL FROM USE

As the notified polymer is used in hair care products it is expected that the entire import volume will be released to the environment via commercial and consumer use (70 and 30%, respectively) and end up in sewers. Some residues will remain in the end user hair care containers.

RELEASE OF CHEMICAL FROM DISPOSAL

After rinsing, imported plastic drums will be sent to landfill. End use containers will be disposed of to domestic garbage and end up in landfill sites.

7.1.2 Environmental fate

Information on the biodegradation of the notified polymer was not provided. Based on its chemical structure, the notified polymer is expected to undergo biodegradation at a slow rate. However, in acclimated biological treatment systems such as sewage treatment plants, removal of quaternary ammonium compounds is generally expected to exceed 90% as a result of sorption and biodegradation (Boethling, 1984). However, studies of quaternary ammonium compounds often do not distinguish between removal due to biodegradation and removal by sorption.

Based on the positive charge and the molecular size of the notified polymer, it is not likely to cross biological membranes and thus absorption is expected to be minimal and bioaccumulation is not expected to occur.

7.1.3 Predicted Environmental Concentration (PEC)

As 70% of the hair care product is expected to be used commercially (313 days/year) and 30% domestically (365 days/year) the average number of days per year where release will occur is calculated to 329 days. The notified polymer contains quaternary imidazolium functional groups. In the calculation of PEC, 90% removal of the notified polymer in STP is assumed, which is the default value for cationic polymers with M_n > 1,000 (Boethling and Nabholz, 1997). Assuming all of the imported volume of the notified polymer is released to the sewer, the PEC of the notified polymer is calculated to be 0.72 µg/L in rivers and 0.07 µg/L in oceans.

Predicted Environmental Concentration (PEC) for the Aquatic Compartment		
Total Annual Import/Manufactured Volume	10 000	kg/year
Proportion expected to be released to sewer	100%	
Annual quantity of chemical released to sewer	10 000	kg/year
Days per year where release occurs	329	days/year
Daily chemical release:	30.4	kg/day
Water use	200.0	L/person/day
Population of Australia (Millions)	21.161	million
Removal within STP	90%	**Mitigation**
Daily effluent production:	4,232	ML
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River:	0.72	µg/L
PEC - Ocean:	0.07	µg/L

7.2. Environmental effects assessment

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

Endpoint	*Result*	*Assessment Conclusion*
Fish Toxicity	LC50 > 20 mg/L	Harmful
Daphnia Toxicity	EC50 > 20 mg/L	Harmful
Algal Toxicity	EC50 > 18 mg/L	Harmful
Inhibition of Bacterial Respiration	IC50 > 200 mg/L	Not harmful

As the ecotoxicity tests were carried out on a maximum of 100 mg/L of the imported product which contains 18 – 21% of the notified polymer, and effects to fish, daphnia and algae were not observed at these levels, the endpoints are conservative. Therefore, worst case, the notified polymer is harmful to fish, aquatic invertebrates and algae. We note the algal test was conducted using media containing humic acid (4 mg/L) which was added to mitigate the toxicity of the test substance. However, measurements of the concentrations of total organic carbon in various humic acid samples in order to determine the toxicity mitigation, as prescribed in Annex 3: Toxicity mitigation testing for cationic substances in OECD (2000), were not reported. Therefore there is doubt about the validity of the determined endpoint for algal toxicity. The notified polymer is not harmful to micro-organisms in the sewage sludge at feasible influent concentrations.

7.2.1 Predicted No-Effect Concentration

Based on the endpoint for the most sensitive trophic level tested (algae) and applying an assessment factor of 100 (3 acute test results are available), the Predicted No-Effect Concentration (PNEC) has been calculated as follows:

Predicted No-Effect Concentration (PNEC) for the Aquatic Compartment		
EC50 (Algae)	> 18	mg/L
Assessment Factor	100	
PNEC:	> 180	µg/L

7.3. Environmental risk assessment

Risk Assessment	PEC µg/L	PNEC µg/L	Q
Q - River	0.72	> 180	**0.004**
Q - Ocean	0.07	> 180	**0.0004**

The Q value (Risk Quotient, PEC/PNEC) to river water has been calculated to be 0.004, based on the worst scenario of assuming all the notified polymer will be released to the aquatic environment. However, doubt has been raised as to the validity of the algal endpoint. Polycationic polyamines which have molecular weights above 1000 and are water soluble are known to be approximately six times more toxic to algae than they are to fish. Assuming the provided algal study is invalid, and based on the above information, an endpoint for algae may be expected to be > 3.3 mg/L. The PNEC derived from this endpoint would be > 3.3 µg/L (using an assessment factor of 1000 since there are less than 3 valid test results). Hence, the Q value to river water is recalculated as 0.22. Therefore, using either of the derived Q values, the notified polymer is not considered to pose an unacceptable risk to aquatic ecosystems based on predicted low PEC/PNEC.

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 polymer in this volume is assumed to infiltrate and accumulate in the top 10 cm of soil (density 1300 kg/m^3). Using these assumptions, irrigation with a concentration of 0.718 µg/L may potentially result in a soil concentration of approximately 5.5 µg/kg. Assuming accumulation of the notified polymer in soil for 5 and 10 years under repeated irrigation, the concentration of notified polymer in the applied soil in 5 and 10 years may be approximately 28 µg/kg and 55 µg/kg, respectively.

8. CONCLUSIONS AND REGULATORY OBLIGATIONS

Hazard classification

Based on the available data the notified polymer is not classified as hazardous under the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)].

and

As a comparison only, the classification of the notified polymer using the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS) (United Nations 2003) is presented below. This system is not mandated in Australia and carries no legal status but is presented for information purposes.

	Hazard category	***Hazard statement***
Environment	Acute Category 3	Harmful to aquatic life

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

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

Environmental risk assessment
On the basis of the PEC/PNEC ratio and the reported use pattern, the notified polymer is not considered to pose a risk to the environment.

Recommendations

CONTROL MEASURES
Occupational Health and Safety

- Employers should implement the following safe work practices to minimise occupational exposure during handling of the imported products containing the notified polymer.
  - Avoid skin and eye contact

- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the imported products containing the notified polymer:
  - Protective eyewear
  - Impervious gloves
  - Protective clothing

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

- A copy of the MSDS should be easily accessible to employees.

- If products and mixtures containing the notified polymer are classified as hazardous to health in accordance with the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)] workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation must be in operation.

Disposal

- The notified polymer should be disposed to landfill.

Emergency procedures

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

Regulatory Obligations

Secondary Notification
This risk assessment is based on the information available at the time of notification. The Director may call for the reassessment of the chemical under secondary notification provisions based on changes in certain circumstances. Under Section 64 of the *Industrial Chemicals (Notification and Assessment) Act (1989)* the notifier, as well as any other importer or manufacturer of the notified chemical, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemical is listed on the Australian Inventory of Chemical Substances (AICS).

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

(1) Under Section 64(1) of the Act; if
- the polymer has a number-average molecular weight of less than 1000;

or

(2) Under Section 64(2) of the Act; if
- the function or use of the chemical has changed from a component of hair styling products at concentrations of up to 2.0%, or is likely to change significantly;
- the amount of chemical being introduced has increased from 10 tonnes, 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 MSDS of products containing the notified chemical provided by the notifier were reviewed by NICNAS. The accuracy of the information on the MSDS remains the responsibility of the applicant.

APPENDIX A: PHYSICAL AND CHEMICAL PROPERTIES

Water Solubility 390 - 480 g/L at 20ºC, pH 7

Method SOP STD/001 from GKA, BASF, SE (Chapter 5: Visual Method)
Remarks Visual Method used to investigate high to complete solubility/miscibility.
Test Facility BASF (2008)

Hydrolysis as a Function of pH Hydrolytically stable

Method OECD TG 111 Hydrolysis as a Function of pH.

pH	*T (°C)*	*$t_{½}$ (years)*
4	50	>1
7	50	>1
9	50	>1

Remarks The hydrolytic stability was investigated using ^{1}H NMR. The test was carried out over 5 days. No significant changes to the ^{1}H NMR spectra after 5 days (including no evidence of formation of degradation products). Given the structure of the notified polymer, it is expected to be hydrolytically stable over environmental pH.
Test Facility BASF (2008)

Partition Coefficient (n-octanol/water) log Pow < -4.9 at 20ºC

Method Estimated from the single solubilities of the notified polymer in water and n-octanol.
Remarks The concentration of the notified polymer in n-octanol was < 5 mg/L and in water > 390 000 mg/L.
Test Facility BASF (2008)

APPENDIX B: TOXICOLOGICAL INVESTIGATIONS

B.1. Acute toxicity – oral

TEST SUBSTANCE	Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).
METHOD	OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method. EC Directive 92/69/EEC B.1tris Acute Oral Toxicity – Acute Toxic Class Method.
Species/Strain	Rat/Wistar HanBrl:WIST(SPF)
Vehicle	Doubly distilled water
Remarks - Method	No significant protocol deviations. GLP compliant.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
I	3 Female	2000	0
II	3 Female	2000	0

LD50	> 2000 mg/kg bw (> 360 – 420 mg/kg bw notified polymer)
Signs of Toxicity	There were no deaths or test substance-related clinical signs during the study period.
Effects in Organs	There were no remarkable necropsy findings.
Remarks - Results	Body weight gains were as expected.
CONCLUSION	The test substance is of low toxicity via the oral route.
TEST FACILITY	BASF (2005a)

B.2. Irritation – skin

TEST SUBSTANCE	Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).
METHOD	OECD TG 404 Acute Dermal Irritation/Corrosion. EC Directive 92/69/EEC B.4 Acute Toxicity (Skin Irritation).
Species/Strain	Rabbit/New Zealand White
Number of Animals	3
Vehicle	None, the test substance was dried for 24 hours prior to administration.
Observation Period	72 Hours
Type of Dressing	Semi-occlusive.
Remarks - Method	No significant protocol deviations. GLP compliant.

RESULTS

Remarks - Results	Mean scores for all animals over 24, 48 and 72 hours was 0.0 for erythema and oedema. Slight erythema was observed in one animal immediately after removal of the patch but not at any later date. No other cutaneous reactions were observed during the study.
CONCLUSION	The notified polymer at a concentration of 18 – 21% is slightly irritating to the skin.
TEST FACILITY	BASF (2005b)

B.3. Irritation – eye

TEST SUBSTANCE Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).

METHOD OECD TG 405 Acute Eye Irritation/Corrosion.
EC Directive 92/69/EEC B.5 Acute Toxicity (Eye Irritation).
Species/Strain Rabbit/New Zealand White
Number of Animals 3 (2 male, 1 female)
Observation Period 72 Hours
Remarks - Method No significant protocol deviations.
GLP compliant.

RESULTS

Lesion	*Mean Score* Animal No.*			*Maximum Value*	*Maximum Duration of Any Effect*	*Maximum Value at End of Observation Period*
	1	2	3			
Conjunctiva: redness	0	0.3	0.3	1	< 48 hours	0
Conjunctiva: chemosis	0	0	0	0	0	0
Conjunctiva: discharge	0	0	0	1	< 24 hours	0
Corneal opacity	0	0	0	0	0	0
Iridial inflammation	0	0	0	0	0	0

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

Remarks - Results No corneal or iridial effects were noted.
No conjunctival chemosis was noted.
A single application of the test material to the non-irrigated eye of the 3 rabbits produced slight conjunctival irritation and discharge 1 hour after treatment in all animals. Two animals continued to show slight conjunctival irritation at the 24 hour observation and no ocular reactions were observed at the 48 hour observation.

CONCLUSION The notified polymer at a concentration of 18 – 21% is slightly irritating to the eye.

TEST FACILITY BASF (2005c)

B.4. Skin sensitisation

TEST SUBSTANCE Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).

METHOD OECD TG 406 Skin Sensitisation – Buehler Test.
EC Directive 96/54/EC B.6 Skin Sensitisation – Buehler Test.
Species/Strain Guinea pig/Hsd Poc: DH (SPF)
PRELIMINARY STUDY Maximum Non-irritating Concentration:
topical: 100% test substance (18 – 21% notified polymer) air dried on patch for 30 mins prior to application.
MAIN STUDY
Number of Animals Test Group: 20 Control Group: 10
INDUCTION PHASE Induction Concentration:
topical: 100% test substance (18 – 21% notified polymer) air dried on patch for 30 mins prior to application.
Signs of Irritation No signs of irritation were seen after the first induction. In the second induction 1/20 animals showed discrete or patchy erythema and in the third induction it was 8/20 animals.
CHALLENGE PHASE
1st challenge topical: 75% test substance (13 – 16% notified polymer)
Remarks - Method Positive control with α-hexylcinnamaldehyde tech. 85%, performed twice a year in laboratory.
No significant protocol deviations.

GLP compliant.

RESULTS

Animal	*Challenge Concentration*	*Number of Animals Showing Skin Reactions after:*			
		1st challenge		*2nd challenge*	
		24 h	*48 h*	*24 h*	*48 h*
Test Group	75%	0/20	0/20	-	-
Control Group	0	0/10	0/10	-	-

Remarks - Results: There were no deaths or test substance-related clinical signs of toxicity or remarkable body weight changes during the study. There were no reactions indicative of sensitisation to the test substance following the challenge exposure.

CONCLUSION: There was no evidence of reactions indicative of skin sensitisation to the notified polymer when tested at a concentration of 18 – 21% under the conditions of the test.

TEST FACILITY: BASF (2005d)

B.5. Genotoxicity – bacteria

TEST SUBSTANCE: Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).

METHOD: OECD TG 471 Bacterial Reverse Mutation Test.
EC Directive 2000/32/EC B.13/14 Mutagenicity – Reverse Mutation Test using Bacteria.
Both the plate incorporation procedure and the pre incubation procedure were conducted.

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

Metabolic Activation System: Rat S9 fraction from aroclor induced rat liver

Concentration Range in Main Test: a) With metabolic activation: 100 – 25,000 µg/plate
b) Without metabolic activation: 100 – 25,000 µg/plate

Vehicle: Water

Remarks - Method: No preliminary test was conducted.
The concentration ranges used were the same for the plate incorporation procedure and the pre incubation procedure.
GLP compliant.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in Preliminary Test	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1		> 25,000	> 25,000	negative
Test 2		> 25,000	> 25,000	negative
Present				
Test 1		> 25,000	> 25,000	negative
Test 2		> 25,000	> 25,000	negative

Remarks - Results

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

TEST FACILITY: BASF (2004a)

B.6. Genotoxicity – in vitro

TEST SUBSTANCE	Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).
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	Chinese hamster V79
Metabolic Activation System	Rat S9 fraction from aroclor induced rat liver
Vehicle	Culture medium
Remarks - Method	No significant protocol deviations. GLP compliant.

Metabolic Activation	*Test Substance Concentration (µg/mL)*	*Exposure Period*	*Harvest Time*
Absent			
Test 1	0*, 1563, 3125, 6250*, 12500*, 25000*	4	18
Test 2a	0*, 390.6, 781.3, 1562.5*, 3125*, 6250*, 12500	18	18
Test 2b	0*, 1562.5, 3125, 6250, 12500*	18	28
Present			
Test 1	0*, 1563, 3125, 6250*, 12500*, 25000*	4	18
Test 2	0*, 1562.5, 3125, 6250*, 12500*, 25000*	4	28

*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	> 25000	> 25000	> 25000	negative
Test 2a	25000	> 12500	> 12500	negative
Test 2b		> 12500	> 12500	negative
Present				
Test 1	> 25000	> 25000	> 25000	negative
Test 2	> 25000	> 25000	> 25000	negative

Remarks - Results	The positive and vehicle controls gave satisfactory responses, confirming the validity of the test system. The test material did not induce any statistically significant increases in the frequency of cells with aberrations.
CONCLUSION	The test substance was not clastogenic to V79 cells treated in vitro under the conditions of the test.
TEST FACILITY	BASF (2006)

APPENDIX C: ENVIRONMENTAL FATE AND ECOTOXICOLOGICAL INVESTIGATIONS

C.1. Ecotoxicological Investigations

C.2.1. Acute toxicity to fish

TEST SUBSTANCE	Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).
METHOD	OECD TG 203 Fish, Acute Toxicity Test – Static, 96 h EC Directive 92/69/EEC C.1 Acute Toxicity for Fish – Static, 96h.
Species	Zebra fish (*Danio rerio*)
Exposure Period	96 h
Auxiliary Solvent	None
Water Hardness	250 mg $CaCO_3$/L
Analytical Monitoring	Polyelectrolyte titration (titrated with polyvinyl sulfate potassium salt; standard curve used)
Remarks – Method	The test was carried out under static conditions. The LC50 was derived from a 96 hour range finding study. The tests were performed with a normal photoperiod of 16 hours at 75 – 236 Lux, a temperature range of 23 – 24ºC and the concentrations of dissolved oxygen were maintained above 60% of the maximum saturation at the test temperature. The fish were observed for survival and toxic signs (changes in appearance, swimming behaviour and behaviour in comparison to a control group). Fish were considered dead if there was no visible movement and no reaction after touching. Dead fish were removed from the test vessels.

RESULTS

Concentration mg/L		*Number of Fish*	*Mortality*				
Nominal	*Actual*		*1 h*	*24 h*	*48 h*	*72 h*	*96 h*
0	<5	10	0	0	0	0	0
100	99	10	0	0	0	0	0

LC50	> 100 mg/L at 24 hours. > 100 mg/L at 48 hours. > 100 mg/L at 72 hours. > 100 mg/L at 96 hours.
NOEC	100 mg/L at 96 hours.
Remarks – Results	No statistical analysis was carried out since no lethality was observed at the highest tested concentration. The endpoints are given as nominal concentrations since these values did not significantly differ from the analytical determinations. Since quantitation was carried out using a standard curve obtained by analysing known concentrations of the test substance and the test substance contains 18 – 21% of the notified polymer, the LC50 of the notified polymer is > 20 mg/L at 96 hours and NOEC = 20 mg/L at 96 hours.
CONCLUSION	The test substance is not harmful to fish. As the notified polymer was only tested to 20 mg/L, it is classified as, at worst, harmful to fish.
TEST FACILITY	BASF (2004b)

C.2.2. Acute toxicity to aquatic invertebrates

TEST SUBSTANCE	Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).
METHOD	OECD TG 202 Daphnia sp. Acute Immobilisation Test and Reproduction Test – Static, 48 h. EC Directive 92/69/EEC C.2 Acute Toxicity for Daphnia – Static, 48 h

Species	*Daphnia magna*
Exposure Period	48 hours
Auxiliary Solvent	None
Water Hardness	220 – 320 mg $CaCO_3$/L
Analytical Monitoring	Polyelectrolyte titration (titrated with polyvinyl sulfate potassium salt; standard curve used)
Remarks - Method	The test was carried out under static conditions. The LC50 range was up to 100 mg/L. The tests were performed with a normal photoperiod of 16 hours, a temperature range of 19.6 – 19.9ºC and the concentrations of dissolved oxygen were >3 mg/L (i.e. 8.8 – 9.3 mg/L) and the pH ranged 8.2 – 8.5. In the control, the immobilisation was ≤10% and no daphnids were captured in a surface film of water. The EC50 (24h) of the control substance, potassium dichromate, was 1.07 mg/L. The test is therefore valid. The daphnids were observed for their swimming ability.

RESULTS

Concentration mg/L		*Number of D. magna*	*Number Immobilised*	
Nominal	*Actual*		*24 h*	*48 h*
0	< 5	5	0	0
12.5	11.5	5	0	0
25	25.5	5	0	0
50	51	5	0	0
100	103.5	5	0	0

EC50	> 100 mg/L at 24 hours > 100 mg/L at 48 hours
NOEC	100 mg/L at 48 hours
Remarks - Results	The EC values are given as nominal concentrations since there is no significant difference between the analytically determined and nominal values. Since quantitation was carried out using a standard curve obtained by analysing known concentrations of the test substance and the test substance contains 18 – 21% of the notified polymer , the LC50 of the notified polymer is > 20 mg/L at 96 hours and NOEC = 20 mg/L at 96 hours.

CONCLUSION The test substance is not harmful to aquatic invertebrates. As the notified polymer was only tested to 20 mg/L, it is classified as, at worst, harmful to aquatic invertebrates.

TEST FACILITY BASF (2004c)

C.2.3. Algal growth inhibition test

TEST SUBSTANCE Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).

METHOD OECD TG 201 Alga, Growth Inhibition Test.
EC Directive 92/69/EEC C.3 Algal Inhibition Test.
EPA Ecological Effects Test Guidelines. OPPTS 850.5400 (Public Draft, April 1996): Algal Toxicity, Tiers I and II.

Species	Green algae (*Desmodesmus subspicatus*)
Exposure Period	72 hours
Concentration Range	Nominal: 0.371, 1.11, 3.33, 10, 30, 100 mg/L Actual: < 10, 22, 89 mg/L (mean values for determinations made at 0 and 72 h)
Auxiliary Solvent	None
Water Hardness	Not provided
Analytical Monitoring	Cell density was measured using the chlorophyll-a-fluorescence method (pulsed excitation with light flashes having a wavelength at 435 nm).

Polyelectrolyte titration (titrated with polyvinyl sulfate potassium salt; standard curve used) was used to measure the concentrations of the test substance in the test solutions and controls.

Remarks - Method

The study was performed under static conditions with an initial cell density of ~ 10^4 cells/mL. The growth media was one of the media specified in OECD TG 201 with humic acid (4 mg/L) added to mitigate the toxicity of the test substance (a deviation to the protocol). However, measurements of the concentrations of total organic carbon in various humic acid samples (0, 10 and 20 mg/L humic acid) in order to determine the toxicity mitigation, as prescribed in Annex 3: Toxicity mitigation testing for cationic substances in OECD (2000), were not reported. Therefore there is doubt raised with respect to the endpoints obtained for this test. A 24 h/day light regime was used with an intensity of 60 – 120 µE/(m^2.s) at a wavelength of 400 – 700 nm. The pH of the solutions ranged 7.9 – 8.2 and the test temperatures ranged 23 ± 2ºC. Three replicates were tested for each of the test substance concentrations and the control. The reference substance used was potassium dichromate. The EC50 values were calculated (linear regression analysis) from the concentration-response relationship. The LOEC was determined by comparing the calculated biomass or growth rate of the various concentration levels with the control. The NOEC was the tested concentration immediately below the LOEC.

RESULTS

Biomass		*Growth*	
*E_bC50** *mg/L at 72 h*	*NOEC** *mg/L*	*E_rC50** *mg/L at 72 h*	*NOEC** *mg/L*
> 89	22	> 89	22

* Results based on mean analytically determined concentrations

Remarks - Results

The biomass in the control cultures increased exponentially by at least a factor of 16 (i.e. a factor of ~50) within the 72 hour test period and the coefficient of variation (CV) for the section by section growth rates was < 35% (i.e. ~4%). The CV of the average growth rates in the replicate controls was up to 8%. Since the measured concentrations deviated markedly from the nominal concentrations, the effect concentration, which is based on the analytically determined concentrations are used. As quantitation was carried out using a standard curve obtained by analysing known concentrations of the test substance and the test substance contains 18 – 21% of the notified polymer , the EC50 values of the notified polymer are > 18 mg/L at 96 hours and NOEC = 4 mg/L at 96 hours.

CONCLUSION

Based on the test results, the test substance is not harmful to algae. As the notified polymer was only tested to 18 mg/L, it is classified as, at worst, harmful to algae. However, the results should be treated with caution due to the uncertainty arising from the deviation to the protocol.

TEST FACILITY

BASF (2005e)

C.2.4. Inhibition of microbial activity

TEST SUBSTANCE

Luviquat Supreme (18 – 21% notified polymer in an aqueous solution).

METHOD

OECD TG 209 Activated Sludge, Respiration Inhibition Test.
EC Directive 88/302/EEC C.11 Biodegradation: Activated Sludge Respiration Inhibition Test

Inoculum

Municipal sewage sludge

Exposure Period

1/2 hour

Concentration Range	Nominal: 248, 496, 1000 mg/L Actual: Not provided
Remarks – Method	Standard protocol was followed. The OECD validity criteria were satisfied. The study was considered to be valid.

RESULTS

IC20	700 mg/L
Remarks – Results	The IC50 result of > 1000 mg/L was determined from extrapolation of the respiration inhibition v nominal concentration curve. Since the test substance contains 18 – 21% of the notified polymer, the IC20 value of the notified polymer is 140 mg/L

CONCLUSION	The notified polymer is not toxic to activated sludge from municipal sewage treatment plants at concentrations < 140 mg/L.
TEST FACILITY	BASF (2004d)

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