File No: LTD/1063

27 March 2003

NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME (NICNAS)

FULL PUBLIC REPORT

Arctical

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Director
Chemicals Notification and Assessment

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1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)
International Flavours & Fragrances (Australia) Ltd (ABN 77 004 269 658) 310 Frankston-Dandenong Rd DANDENONG VIC 3175.

NOTIFICATION CATEGORY
Limited-small volume: Chemical other than polymer, (1 tonne or less per year).

EXEMPT INFORMATION (SECTION 75 OF THE ACT)
The following details are claimed exempt from publication: chemical name, CAS No., molecular and structural formulae, molecular weight and spectral data.

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)
Variation to the schedule of data requirements is claimed as follows: hydrolysis as a function of pH, autoignition temperature and explosive properties.

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)
None.

NOTIFICATION IN OTHER COUNTRIES
USA, Canada and EU (2002).

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)
Arctical

MOLECULAR WEIGHT
< 500

METHODS OF DETECTION AND DETERMINATION

ANALYTICAL METHOD GC analysis, UV, NMR and IR spectroscopy.

3. COMPOSITION

DEGREE OF PURITY
97.5%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS
None.

NON HAZARDOUS IMPURITIES/RESIDUAL MONOMERS (>1% by weight)

Chemical Name 4 unidentified chemicals.
CAS No. *Weight %* 2.4%

ADDITIVES/ADJUVANTS

Chemical Name	2,6-di-t-butyl-4-methyl phenol		
CAS No.	128-37-0	*Weight %*	0.1%

4. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
In 200 L drums as a component (up to 0.2%) of a fragrance oil.

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

Year	*1*	*2*	*3*	*4*	*5*
Tonnes	100 kg	100 kg	100 kg	100 kg	100 kg

USE
The fragrance oil in which the notified chemical is a component of will be used in cosmetics and household products. Final products and weight fraction of the notified chemical include:

Products	Weight Fraction	Products	Weight Fraction
Body lotion	0.00001	Surface cleaners	0.00001
Creams	0.000006	Deodorant sprays	0.00002
Sun creams/lotions	0.000008	Air fresheners (sprays)	0.0001
Hairsprays	0.00001	Soap bars	0.000026
Shampoos	0.00001	Foam baths	0.00004
Dishwashing liquid	0.00001	Toilet waters	0.000154
Fabric washing liquid	0.00001		

5. PROCESS AND RELEASE INFORMATION

5.1. Distribution, Transport and Storage

PORT OF ENTRY
Not stated.

IDENTITY OF MANUFACTURER/RECIPIENTS
Large manufacturers of toileteries, air fresheners, surface cleaners, dish washing and fabric washing liquid.

TRANSPORTATION AND PACKAGING
Importation of drums will be by ship in containers. Products containing the notified chemical would normally be packing in a variety of containers for consumer use and shipped in cardboard cartons by road to retailers.

5.2. Operation Description

Production of the consumer products would be undertaken typically in large manufacturing plants. Mixing vessels can be open or closed depending on the product and local exhaust ventilation is normally employed to reduce exposure to fumes and aerosols. The fragrance oil would normally be pumped from the drum to the mixing vessel or to a vessels in a weighing room. Products would normally be packed automatically again with exhaust ventilation if necessary.

5.3. Occupational exposure

Number and Category of Workers

Category of Worker	*Number*	*Exposure Duration*	*Exposure Frequency*
Mixer	5	4 hours/day	2 days/year
Drum handling	5	"	"
Drum cleaning/washing	10	"	"
Maintenance	5	"	"

QC	2	0.5 hours/day	"
Packaging	10	4 hours/day	"

Exposure Details
The notified chemical is introduced at a concentration of 0.2% in a fragrance oil and diluted to between 0.0006 and 0.0154%.

Transport and storage workers should only be exposed to the fragrance oil in the event that drums are accidentally breached.

The products to which the fragrance oil is added are typically produced in large batches of several thousand litres and the mixing vessels can be open or closed. Hazardous components of the products and the size of the batches usually necessitate the use of closed lines, local exhaust ventilation where vapours or aerosols are produced and automated packing lines. It is common in large plants for the process workers to employ protective clothing, gloves and safety goggles. Exposure to the notified chemical at a maximum of 0.2% would most likely occur when the fragrance oil is pumped to the mixing vessels or to a weighing vessel and drips or spills occur. A maximum of 50 L of fragrance oil would be used in any one batch and the typical amount would be somewhat less. Once in the mixing vessel exposure would be lower and this applies to cleaning of the machinery and lines.

Laboratory technicians and maintenance workers would normally be potentially exposed to low concentrations of the notified chemical and would normally employ personal protective equipment to protect against hazards of other components of the products.

5.4. Release

RELEASE OF CHEMICAL AT SITE
Customers of the notifier will blend the fragrance oil at a maximum percentage of 0.2% into a range of cosmetic and household products at their facilities. It is expected that less than 10 kg per annum of the notified chemical will remain in the empty import containers, which, are likely to be rinsed, and the rinseate either added into the production of the next batch or released into the sewer. The cleaned import containers will either be recycled or disposed of in landfill. Release to the environment during reformulation and cleaning processes are expected to be small as closed, automated systems are used, and will total less than 1 kg (1% of the total fragrance oil mixture) per annum of the notified chemical. Wastes from these processes will be disposed of in either landfill or into the sewer

RELEASE OF CHEMICAL FROM USE
Since the notified chemical will be used in household, laundry and personal cleaning products, up to 98 kg per annum is expected to be released to sewer. The release from the chemical remaining in the consumer product containers is expected to be in low amounts. These containers, which will vary in size and construction material, will be disposed of into domestic rubbish and ultimately landfill. The material of construction of these containers may be glass, plastic, metal or paperboard.

5.5. Disposal
The majority of the notified chemical will ultimately be disposed of to sewer. Spilt material will be contained by absorbent, placed into containers and disposed in landfill.

5.6. Public exposure
Public exposure to the notified chemical as imported at a concentration of up to 0.2% in fragrance oil could occur in the event of a transport accident. Public exposure from the formulation process is unlikely but exposure to the consumer products containing the notified chemical at a maximum concentration of 0.0154% will be widespread.

6. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa Colourless to pale yellow liquid.

Melting Point/Freezing Point < 20°C

METHOD EC Directive 92/69/EEC A.1 Melting/Freezing Temperature.

Remarks
TEST FACILITY Safepharm (2001).

Boiling Point 221°C at 101.3 kPa

METHOD EC Directive 92/69/EEC A.2 Boiling Temperature.
Remarks
TEST FACILITY Safepharm (2001).

Density 807 kg/m^3

Vapour Pressure 0.0251 kPa at 25°C.

Remarks An estimated boiling point value of 231.35°C (by the adapted Stein and Brown Method) was used to estimate the vapour pressure using MPBPWIN v1.40. Three vapour pressure estimates were derived using the Antoine Method, Modified Grain Method and Mackay Method and the mean of the results of the Antoine and Grain methods was selected (0.113 mm Hg).

The Henry's Law constant (H) was calculated from the molecular weight, the measured water solubility, and the estimated vapour pressure according to the following equation: H = MW (g/mol) x Vapour Pressure (Pa)/Water Solubility (mg/L).

H = 305.8 Pa m^3/mol, indicating the substance is volatile (Mensink *et al*. 1995).

Water Solubility < 1.51 × 10^{-5} g/L at 20°C

METHOD EC Directive 92/69/EEC A.6 Water Solubility.
Remarks The water solubility was determined using the flask method. An excess of the notified chemical (~ 110 mg) was added to each of three conical flasks and to each was added double distilled water (100 mL). The flasks were shaken at 30°C and then equilibrated at 20°C for 24 hours. After equilibration, the flask contents were centrifuged, a sample was taken and analysed HPLC. The preliminary water solubility test indicated that the column elution method should have been performed as the solubility was less than 1 × 10^{-2} g/L. However, it was not possible to determine the water solubility via this method because the liquid test substance would coat the glass beads causing them to adhere to each other and prevent circulation of water through the column.
TEST FACILITY Safepharm (2001).

Hydrolysis as a Function of pH Not determined.

Remarks The notified chemical is susceptible to hydrolysis under extremely acidic conditions. Therefore, in the environmental pH range of 4-9, significant hydrolysis is unlikely to occur.

Partition Coefficient (n-octanol/water) log Pow at 20°C = > 6.2 (HPLC Method)

METHOD EC Directive 92/69/EEC A.8 Partition Coefficient.
Remarks The notified chemical exhibited a HPLC retention time that was greater than that of the DDT reference standard. The low water solubility is consistent with the high log Pow, indicative of partitioning into the organic phase.

The notifier has also supplied a calculated log Kow value (by WSKOW v1.40) of 4.76 which in turn allowed a water solubility estimate of 4.5 mg/L, very much higher than that determined experimentally.
TEST FACILITY Safepharm (2001).

Adsorption/Desorption Log Koc = 2.77

Remarks	This value does correspond to that obtained from QSAR modelling data provided by the notifier (PCKOWIN v1.66). The notified chemical has a low water solubility, a high log Pow and a relatively high log Koc indicating a high affinity for the organic component of soils and sediments.

Dissociation Constant Not determined.

Remarks	The notified chemical does not contain any groups capable of dissociation.

Particle Size Not applicable for a liquid.

Flash Point 91°C at 101.3 kPa

METHOD	EC Directive 92/69/EEC A.9 Flash Point.
TEST FACILITY	Safepharm (2002a).

Flammability Limits Not expected to be flammable.

Autoignition Temperature Not done.

Explosive Properties Not done.

Reactivity Not expected to be reactive.

7. TOXICOLOGICAL INVESTIGATIONS

Endpoint and Result	*Assessment Conclusion*
Rat, acute oral LD50 > 2500 mg/kg bw	low toxicity
Rabbit, skin irritation	moderately irritating
Rabbit, eye irritation	slightly irritating
Guinea pig, skin sensitisation - adjuvant test.	no evidence evidence of sensitisation
Human repeated insult patch test	no evidence evidence of sensitisation
Genotoxicity - bacterial reverse mutation	non mutagenic

7.1. Acute toxicity – oral

TEST SUBSTANCE Notified chemical.

METHOD OECD TG 423 Acute Oral Toxicity – Acute Toxic Class Method.
EC Directive 96/54/EEC B.1tris Acute Oral Toxicity – Acute Toxic Class Method.
Species/Strain Rat/Sprague-Dawley.
Vehicle None.

RESULTS

Group	*Number and Sex of Animals*	*Dose mg/kg bw*	*Mortality*
1	5/sex	2000	0/10

LD50 > 2500 mg/kg bw
Signs of Toxicity None.
Effects in Organs None.

CONCLUSION The notified chemical is of low toxicity via the oral route.

TEST FACILITY Safepharm (2002c).

7.2. Irritation – skin

TEST SUBSTANCE Notified chemical.

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.
Observation Period 14 days.
Type of Dressing Semi-occlusive.

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	2	2	2	2	14 days[a]	0
Oedema	2	2	2	2	7 days	0

*Calculated on the basis of the scores at 24, 48, and 72 hours for EACH animal.
[a] moderate desquamation in 2 animals; crust formation in one animal

CONCLUSION The notified chemical is moderately irritating to skin.

TEST FACILITY Safepharm (2002d).

7.3. Irritation - eye

TEST SUBSTANCE Notified chemical.

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
Observation Period 72 hours.

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	0	1	1 hour	0
Conjunctiva: chemosis	0	0	0	1	1 hour	0
Conjunctiva: discharge	0	0	0	1	1 hour	0
Corneal opacity	0	0	0	0		0
Iridial inflammation	0	0	0	0		0

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

Remarks - Results

CONCLUSION The notified chemical is slightly irritating to the eye.

TEST FACILITY Safepharm (2002e).

7.4. Skin sensitisation

TEST SUBSTANCE Notified chemical.

METHOD OECD TG 406 Skin Sensitisation – Maximisation test.
EC Directive 96/54/EC B.6 Skin Sensitisation - Maximisation test.
Species/Strain Guinea pig/Dunkin Hartley.
Vehicle Arachis oil B.P.
PRELIMINARY STUDY Maximum Non-irritating Concentration:
intradermal: < 1% v/v
topical: 100% at > 24 hours
MAIN STUDY
Number of Animals Test Group: 10 Control Group: 5
INDUCTION PHASE Induction Concentration:
intradermal injection: 5% v/v
topical application: undiluted
Signs of Irritation Moderate erythema at intradermal induction sites, slight to moderate erythema at 1 hour and nil to slight erythema at 24 hours after removal of patches for topical induction.
CHALLENGE PHASE
1st challenge topical application: 75% v/v
topical application: 100% v/v

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%	0/10	0/10		
	100%	2/10	0/10		
Control Group	75%	0/5	0/5		
	100%	0/5	0/5		

Remarks - Results: Two animals challenges with neat test substance displayed discrete or patchy erythema. As this did not occur at 48 hours, it did not conclusively indicate skin sensitisation.

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

TEST FACILITY: Safepharm (2002f).

7.5. 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: WP2 uvrA.

Metabolic Activation System: Phenobarbitone/β-naphthoflavone-induced rat liver S9 microsomal fraction.

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

Vehicle: Acetone.

RESULTS

Metabolic Activation	*Test Substance Concentration (µg/plate) Resulting in:*			
	Cytotoxicity in PreliminaryTest	*Cytotoxicity in Main Test*	*Precipitation*	*Genotoxic Effect*
Absent				
Test 1	None.	None.	5000	Negative
Test 2		None.		Negative
Present				
Test 1	None.	None.	5000	Negative
Test 2		None.		Negative

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

TEST FACILITY: Safepharm (2002g).

ADDITIONAL INVESTIGATIONS

7.13T. Skin sensitisation – human volunteers

TEST SUBSTANCE	Notified chemical.
METHOD	
Study Design	Repeated insult patch test.
Study Group	Twenty-four males and 86 females ranging in age from 18 to 69 years. 101/110 subjects successfully completed the test procedure.
Vehicle	None.
Induction Procedure	Approximately 0.2 mL of the test substance (1% Arctical in alcohol SD39C:DEP(75:25)) was placed under an occlusive patch for 24 hours.
Rest Period	In each week there were 2 rest periods of 24 hours then 1 rest period of 48 hours for a total of 9 applications.
Challenge Procedure	After a rest period of approximately 14 days, the challenge patch (1% Arctical in alcohol SD39C:DEP(75:25)) was applied and the site scored 24 and 72 hours later.
CONCLUSION	The notified chemical was non-irritating and non-sensitising/sensitising under the conditions of the test.
TEST FACILITY	Essex Testing Clinic (2002).

8. ENVIRONMENT

8.1. Environmental fate

8.1.1. Ready biodegradability

TEST SUBSTANCE

METHOD	OECD TG 301 B Ready Biodegradability: CO_2 Evolution Test.
Inoculum	Activated sludge
Exposure Period	28 days
Auxiliary Solvent	none
Analytical Monitoring	

RESULTS The notified chemical was incubated for 28 days at a test substance concentration of 12.8 mg/L.

Test substance		*Sodium Benzoate*	
Day	*% degradation*	*Day*	*% degradation*
14	23	14	68
28	29	28	83

Remarks - Results The biodegradation of the reference substance, sodium benzoate was 83% after 28 days, indicating the test conditions were valid. After 28 days at 21°C, the test substance underwent 29% biodegradation which indicates the notified chemical is not readily biodegradable in aerobic environments. The test substance was also found to be non-inhibitory to micro-organisms.

CONCLUSION The notified chemical is not readily biodegradable.

TEST FACILITY Safepharm (2002b).

8.1.2. Bioaccumulation

Data regarding the bioaccumulation potential of the notified chemical were not provided for this notification. However, the notifier has provided a calculated bioconcentration factor value (by BCFWin) of 92.79 (log BCF = 1.97) based on a calculated partition coefficient of 4.76. The value provided is a calculated value based on another calculated value and, as such, should be treated with caution. The chemical structure, molecular weight, water solubility, and Pow suggest a potential for the notified chemical to cross biological membranes and bioaccumulate (Connell 1990). However, the low import volume and dispersed use suggest exposure will not be significant.

8.2. Ecotoxicological investigations

No ecotoxicity data were submitted. However, the notifier has provided QSAR modelling that suggests that the class of chemical to which the notified chemical belongs is expected to exhibit the following toxicities to aquatic organisms.

Daphnia (48 h LC50)	0.424 mg/L
Algae (96 h EC50)	0.243 mg/L

These estimated values should be treated with extreme caution as they were based on a calculated water solubility of 1.254 mg/L (cf. 1.51×10^{-2} mg/L experimentally determined and 4.5 mg/L calculated separately – see above)

9. RISK ASSESSMENT

9.1. Environment

9.1.1. Environment – exposure assessment

Exposure

The notified chemical is volatile (0.0251 kPa at 25°C) and loss to the atmosphere is likely to be a relatively significant process from surfaces to which the fragrance oil is applied, sewers, aquatic and terrestrial environments. In environments where volatilisation to the atmosphere is not able to occur (eg. deep waters, groundwater, subsoils), the notified chemical is expected to be relatively persistent. It is not readily biodegradable but will likely biodegrade over time as the notified chemical attained 29% degradation after 28 days and it would likely have degraded further with more time. The notified chemical will not readily hydrolyse in natural waters at environmentally-relevant pH values. It is very slightly soluble in water (< 1.51×10^{-5} mg/L; Mensink et al., 1995) so has a potential to adsorb to particulate organic material and therefore accumulate in sediments due to this sorption and settlement. It is not expected to be very mobile in soils and groundwaters due to its low sorption potential (Log Koc 2.77) and low water solubility.

The main fate pathways for the notified chemical following its uses in Australia include dissipation in air due to its volatility, but a large proportion has the potential to be discharged into sewage treatment systems following its use, and there is a potential for discharges from these systems to aquatic environments to contain the notified chemical (refer below). Relatively minor quantities may potentially be released during formulation, storage, handling and transportation, (eg. uncontained spills and leaks) resulting in discharges to land, aquatic environments; however, the majority of the wastes generated are expected to be discharged to sewer or sent to landfills for disposal.

In landfills, the notified chemical may occur in residues in disposed emptied containers or in sludges derived from wastewater treatment plants and formulation and drum recycling facilities. These residues may potentially constitute only a fraction of the total product (eg. ~3% of 0.3 kg of the notified chemical per annum). Over time, residues of the notified chemical in containers and unstabilised sludges may dissolve and mobilise in leachate. However, sorption to organic matter may occur and biodegradation of the notified chemical is likely over time.

Australia has a population of approximately 19.5 million people, and an average value for water consumption of 200 L/person/day has been adopted for this national-level assessment (3900 ML/day for total population). Therefore, the concentration of notified chemical in the Australian sewerage network may approximate 7×10^{-5} mg/L (ie. 1×10^{8} mg ÷ 365 days/year ÷ 3900×10^{6} L; 0.07 μg/L), assuming that 100% of the notified chemical remains in the aqueous compartment. Based on dilution factors of 0 and 10 for inland and ocean discharges of STP-treated effluents, outfalls, predicted environmental concentrations (PECs) of the notified chemical in freshwater and marine surface waters may approximate 0.07 μg/L and 0.007 μg/L, respectively.

Using a worst case scenario, it has been assumed that all of the notified chemical used is discharged sewerage systems throughout Australia. Using the SIMPLETREAT model for modelling partitioning and losses in sewage treatment plants (STPs; European Commission, 1996), the percent removal by STPs may potentially approximate 91.5% (eg. 91.5 kg) of the quantity entering the STPs, with approximately 16% (eg. 16 kg) released to air through volatilisation, and approximately 75.5% (eg. 75.5 kg) partitioned to sludge. Approximately 8.5% (eg. 8.5 kg) of the inflow concentration of the notified chemical may potentially remain in solution, passing through the STP. These partition estimates assume that no degradation of the notified chemical occurs during the STP process. Release to sewer of 8.5 kg of the notified chemical now gives PECs in freshwater and marine surface waters of 0.006 μg/L and 0.0006 μg/L), respectively.

Partitioning to biosolids in STPs Australia-wide may result in an average biosolids concentration of 0.19 mg/kg (dry wt). Effluent re-use concentration may potentially approximate 6×10^{-5} mg/L.

Biosolids are applied to agricultural soils, with an assumed average rate of 10 t/ha/year. Assuming a soil bulk density of 1000 kg/m^3 and a soil mixing zone of 0.1 m, the concentration of the notified chemical may approximate 0.0019 mg/kg in applied soil. This assumes that degradation of the notified chemical occurs in the soil within 1 year from application. Assuming accumulation of the notified chemical in soil for 5 and 10 years under repeated biosolids application, the concentration of notified chemical in the applied soil in 5 and 10 years may approximate 0.0095 mg/kg and 0.019 mg/kg, respectively.

STP effluent re-use for irrigation in Australia 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 0.1 m of soil (density 1000 kg/m^3). Using these assumptions, irrigation with a concentration of 6×10^{-5} mg/L may potentially result in a soil concentration of approximately 6×10^{-4} mg/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 approximate 0.003 mg/kg and 0.006 mg/kg, respectively.

Fate
When released to sewer, the notified chemical is expected to adsorb to soil/sediment particles and degrade slowly to water vapour and oxides of carbon through biotic and abiotic processes.

Residual chemical disposed of into landfill with empty containers or with residual solids derived from water treatment at the production facilities is also expected to remain adsorbed to soil/sediment particles, and in this situation would be expected to be slowly destroyed by similar mechanisms to those operating in sediments. Incineration of the material would produce water vapour and oxides of carbon and nitrogen.

As indicated above, approximately 16 kg of the notified chemical will volatilise into the air. Here, according to modelling data provided by the notifier (AOP v1.9) degradation of the notified chemical in the atmosphere is expected to occur through hydrogen abstraction by hydroxy radicals, with half-lives for the cis- and trans-isomers of 1.442 and 1.298 h, respectively.

9.1.2. Environment – effects assessment

The modelled results for ecotoxicity indicate the notified substance is very toxic to both Daphnia and algae. The most sensitive species are expected to be algae, where the 72 hour EC50 is calculated to be 0.243 mg/L.

Since only two estimated results are available, applying an assessment factor of 1000 to the most sensitive species (algae), the predicted no effects concentration (PNEC) is 0.243 µg/L.

9.1.3. Environment – risk characterisation

Table 1: PEC/PNEC Ratios for nation-wide use based on an import volume of 100 kg per annum and assuming no removal from the aqueous compartment.

Location	PEC	PNEC	PEC/PNEC Ratio
Ocean outfall	0.007 µg/L	0.243 µg/L	0.029
Inland River	0.07 µg/L	0.243 µg/L	0.29

Table 2: PEC/PNEC Ratios based on an import volume of 100 kg per annum based on nation wide use calculated assuming 8.5% of the notified chemical partitioned into water and 91.5% is removed during the STP process based on SIMPLETREAT model.

Location	PEC	PNEC	PEC/PNEC Ratio
Ocean outfall	0.0006 µg/L	0.243 µg/L	0.0024
Inland River	0.006 µg/L	0.243 µg/L	0.024

Table 3: PEC/PNEC Ratios based on an import volume of 1000 kg per annum (ie. The import limit allowed under a Limited Notification) based on nation wide use and assuming no removal from the aqueous compartment.

Location	PEC	PNEC	PEC/PNEC Ratio
Ocean outfall	0.07 µg/L	0.243 µg/L	0.29

Inland River	0.7 µg/L	0.243 µg/L	**2.9**

The new chemical will be used as a fragrance ingredient of domestic cleaning and personal care formulations, and most will eventually be released into domestic sewage systems as a consequence of product use. The compound is not readily biodegradable (29% over 28 days), and has a high partition coefficient of greater than 6.2 and a low water solubility ($<1.51 \times 10^{-5}$ mg/L), all indicating that most of the material would eventually partition to sediment. Here it is expected to slowly degrade to water and oxides of carbon through biological processes.

It should be noted that much of the physico-chemical data provide in the submission has been generated by QSAR modelling and that in certain circumstance several different values have been calculated for partition coefficient and water solubility. Given that these physico-chemical values form the basis of the calculation for determining Henry's Law constant (H) and from that the proportions partitioned into each environmental compartment using the SIMPLETREAT model, these partitioning values should be treated with caution.

Assuming a worst case situation where the entire import volume of 100 kg is released to sewer and remains in the aqueous compartment, the PEC/PNEC ratio for the aquatic environment, assuming nationwide use, is 0.29 (Table 1). This value is less than 1, indicating no immediate concern to the aquatic compartment.

However under a Limited notification, the notifier is entitled to import up to 1000 kg per annum. Assuming an increase in import volume to this level and complete release to sewer without removal of the notified chemical from the aqueous compartment (see comment above), the PEC is now 0.7 µg/L, giving a PEC/PNEC ratio for the aquatic environment of 2.9 (Table 3). This value is significantly greater than 1, indicating an immediate concern to the aquatic compartment.

However, the above considerations indicate minimal hazard to the environment when the new chemical is used as a component of domestic cleaning and personal care products in the manner and levels (< 100 kg and removal from STP; Table 2) indicated by the notifier.

9.2. Human health

9.2.1. Occupational health and safety – exposure assessment

The notified chemical will be imported as a 0.2% component of a fragrance oil in 200 L drums. For each batch of product a fraction of the drum contents would be weighed out or metered directly into the mixing vessel. Typically local exhaust ventilation is used to control exposure to fumes and gloves, goggles and protective clothing are used to control exposure to drips and spills which would be expected to occur intermittently. Once the fragrance oil is in the mixing vessel the process is automated and exposure of workers is unlikely. Quality control, maintenance and cleaning workers may be exposed to very low concentrations of the notified chemical in final products.

9.2.2. Public health – exposure assessment

The public would normally be exposed to the notified chemical at a maximum concentration of 0.0154% but exposure can be extensive when various toiletries are used. If it assumed that 0.8 g of toilet water is applied up to 5 times per day and there is 100% uptake, the dosage for a 60 kg person would be 0.01 mg/kg/day.

9.2.3. Human health - effects assessment

The notified chemical is of low acute oral toxicity in rats, is a moderate skin irritant in rabbits, a slight eye irritant in rabbits, is not a skin sensitiser in humans or guinea pigs and is not mutagenic in bacteria.

The notified chemical would be classified as a hazardous substance according to the NOHSC *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 1999) and assigned the risk phrase R38: Irritating to skin.

9.2.4. Occupational health and safety – risk characterisation

The notified chemical is unlikely to be acutely toxic, irritant to eyes, sensitising or genotoxic. It

is irritating to skin but the imported product would not be classified as a skin irritant solely on the basis of the content of the notified chemical which is low, at 0.2% of the imported fragrance oil.

Exposure of workers involved in reformulation, QC, maintenance and end use is likely to be low and intermittent further reducing the risk of adverse health effects. Therefore, the risk of adverse health effects to workers handling the imported fragrance oil is judged to be low.

9.2.5. Public health – risk characterisation

There is a possibility of public exposure in the event of a transport accident but the risk of skin irritation from subsequent skin contact with domestic products is low.

Repeated use of domestic products containing the notified chemical is unlikely to elicit skin irritation given that its maximum concentration in these products is 0.0154%.

10. CONCLUSIONS – ASSESSMENT LEVEL OF CONCERN FOR THE ENVIRONMENT AND HUMANS

10.1. Hazard classification

Based on the available data the notified chemical is classified as hazardous under the NOHSC *Approved Criteria for Classifying Hazardous Substances*. The classification and labelling details are:

R38: Irritating to skin.

10.2. Environmental risk assessment

The chemical is not considered to pose a risk to the environment based on its reported use pattern and at an import volume of no greater than 100 kg per annum.

10.3. Human health risk assessment

10.3.1. Occupational health and safety

There is Low Concern to occupational health and safety under the conditions of the occupational settings described.

10.3.2. Public health

There is Negligible Concern to public health when used as described.

11. MATERIAL SAFETY DATA SHEET

11.1. Material Safety Data Sheet

The MSDS of the notified chemical provided by the notifier was in accordance with the NOHSC *National Code of Practice for the Preparation of Material Safety Data Sheets* (NOHSC, 1994a). It is published here as a matter of public record. The accuracy of the information on the MSDS remains the responsibility of the applicant.

11.2. Label

The label for the notified chemical provided by the notifier was in accordance with the NOHSC *National Code of Practice for the Labelling of Workplace Substances* (NOHSC, 1994b). The accuracy of the information on the label remains the responsibility of the applicant.

12. RECOMMENDATIONS

REGULATORY CONTROLS
Hazard Classification and Labelling

- The NOHSC Chemicals Standards Sub-committee should consider the following health hazard classification for the notified chemical:
  - R38: Irritating to skin

- Use the following risk phrases for products/mixtures containing the notified chemical:

  Products containing ≥ 20% R38

CONTROL MEASURES
Occupational Health and Safety

- Employers should implement the following engineering controls to minimise occupational exposure to the notified chemical as introduced:
  - Local exhaust ventilation, closed blenders

- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical during formulation of the fragrance concentrate and consumer products:
  - Chemical resistant gloves, protective overalls, and goggles/faceshield.

  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 chemical are classified as hazardous to health in accordance with the NOHSC *Approved Criteria for Classifying Hazardous Substances*, workplace practices and control procedures consistent with provisions of State and Territory hazardous substances legislation must be in operation.

Environment

- The following control measures should be implemented by end users to minimise environmental exposure during use of the notified chemical:
  - Do not allow material or contaminated packaging resulting from spills to enter drains, sewers or water courses.

Disposal

- The notified chemical should be disposed of to landfill where practicable.

Emergency procedures

Gross spills/release of the notified chemical should be contained by sand or inert powder and earth. Collect and seal in properly labelled drums for disposal in landfill.

12.1. Secondary notification

The Director of Chemicals Notification and Assessment 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 import volume increases above 250 kg per annum, the notifier should provide results and test reports for vapour pressure, adsorption/desorption, hydrolysis as a function of pH and aquatic ecotoxicity data for fish, Daphnia and algae for the notified chemical or quantitative data on removal of the chemical in sewage treatment plants.

(2) Under subsection 64(2) of the Act:

– if any of the circumstances listed in the subsection arise.

The Director will then decide whether secondary notification is required.

No additional secondary notification conditions are stipulated.

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