

File No: LTD/1263

3 August 2006

**NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME
(NICNAS)**

FULL PUBLIC REPORT

Control Agent 3358

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 and Heritage.

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**Director
NICNAS**

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FULL PUBLIC REPORT

Control Agent 3358

1. APPLICANT AND NOTIFICATION DETAILS

APPLICANT(S)

Orica Limited (ABN: 24 004 145 868)
1970 Princes Highway
Clayton VIC 3168

NOTIFICATION CATEGORY

Limited-site limited: Chemical other than polymer, (10 tonnes or less per year).

EXEMPT INFORMATION (SECTION 75 OF THE ACT)

Data items and details claimed exempt from publication:

Chemical name

Other name(s)

CAS number

Molecular formula

Structural formula

Molecular weight

Spectral data

Purity

Methods of detection and determination

Volume

Identity of sites

VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)

Variation to the schedule of data requirements is claimed as follows:

Boiling point

Vapour pressure

Flash point

Explosive properties

PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)

None

NOTIFICATION IN OTHER COUNTRIES

None

2. IDENTITY OF CHEMICAL

MARKETING NAME(S)

Control Agent 3358

METHODS OF DETECTION AND DETERMINATION

METHOD	The solid chemical may be most conveniently characterised by ^1H NMR or infrared spectroscopy.
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3. COMPOSITION

DEGREE OF PURITY
>99%

HAZARDOUS IMPURITIES/RESIDUAL MONOMERS
None

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

ADDITIVES/ADJUVANTS
None

DEGRADATION PRODUCTS
Metabolic breakdown of the notified chemical is likely to involve reduction and cleavage of the functional group. The reaction is likely to be catalysed by enzymes.

The notified chemical is expected to undergo thermal degradation at approximately 200 °C.

Degradation of the notified chemical may result in the formation of carbon disulfide.

4. INTRODUCTION AND USE INFORMATION

MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS
The notified chemical will be manufactured in Australia.

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

<i>Year</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>
<i>Tonnes</i>	1-3	1-3	3-10	3-10	3-10

USE
The notified chemical will be used as a chain transfer agent during the polymerisation of styrene/acrylic monomers. It will be present at a concentration of <20% for the polymerisation process. The polymer containing the notified chemical has been assessed by NICNAS and will be used as an additive in the manufacture of water borne latex that will then be formulated into paint.

5. PROCESS AND RELEASE INFORMATION

5.1. Distribution, transport and storage

IDENTITY OF MANUFACTURER/RECIPIENTS
The manufacturing site is located in Melbourne, Victoria.

TRANSPORTATION AND PACKAGING
The material will be stored in 20 L containers on-site.

5.2. Operation description

Manufacture

The reactants are charged in various stages to a 400 L batch reactor over a period of three hours in order to manufacture the notified chemical. The raw materials are all liquids that are pumped in from 200 L drums. Those that are particularly toxic are pumped in from a dedicated sealed booth to avoid worker exposure. The reactor is equipped with an agitator and a chilled water condenser. Temperature control (ambient temperature of approx 25-30 °C) is achieved by application of steam or chilled water to a jacket surrounding the reactor. The batch reaction provides 50 kg of the notified chemical. The major unit operation steps involved in the manufacture are as follows:

Brief operation	Detailed operation description	Points of release and mass of
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description		material
Reactant charging	Reactants are pumped into the reactor and stirred	
pH sample	Sample taken and the pH checked in the QC lab	Sample (~50 grams)
Separation	Lower aqueous layer separated from upper acetone/notified chemical layer	Notified chemical present in aqueous layer drained into drums (less than 1 gram)
Solvent removal	Acetone is distilled from the reaction mixture under vacuum	
Filtration	A slurry of the chemical is filtered	Notified chemical collected on filter cloth (approx. 50 kg) Notified chemical lost in filtrate (less than 1 gram)
Reactor rinsing	The reactor is rinsed with water to dislodge any solid notified chemical remaining on walls	Notified chemical rinsed into filter (approx. 200 grams)
Washing	The filter cake is washed with heptane	Notified chemical loss in filtrate (approx. 240 grams)
Solids samples	Samples are taken and evaluated for their solids content in the QC lab	Samples (approx. 100 grams in total)
Packaging	The solid product is carefully scooped into containers.	Notified chemical left on filter bag. (approx. 200 grams)
Reactor washing	The reactor is washed by boiling with water	Minimal residue washed away to on-site aqueous waste ponds (less than 10 grams)

Use in polymer preparation

The notified chemical is used in the preparation of a copolymer of styrene and/or acrylic monomers. In a typical process the notified chemical is combined with a free radical initiator in propylene glycol and heated in a stirred 2000 L batch reactor. Monomers are then added and polymerisation is allowed to proceed over an eight hour period. The final solution of polymer is then discharged to bulk storage containers and transported to a site where it is used as an additive in waterborne latex manufacture.

5.3. Occupational exposure

Nature of Work and Number and Category of Workers

Work Type	Nature of Work	No. Exposed	Exposure hrs/day	Exposure Days/year
<u>Manufacture</u>				
Reactor operators	Charging raw materials, processing, filling, collection of QC samples	2	5	20
Maintenance personnel	Repair reactor vessel, transfer lines, pumps, mixers, etc	2	1–2	20
Laboratory personnel	Testing of QC samples, troubleshooting	2	2	20
Storage and internal transport personnel	Storage of finished product in containers.	2	2	20
<u>Use in polymerisation</u>				
Reactor operators	Charging as a raw material.	1	1	20

Exposure Details

The notified chemical is in powder form at each stage during its handling. As such, there is the potential for workers to be exposed to airborne dust via skin, eyes or by inhalation, particularly when adding the notified chemical to the batch reactor for the subsequent polymerisation process. However, dermal and inhalation exposure should be minimised by the use of local exhaust ventilation and appropriate personal protective equipment (chemical gloves, coveralls, goggles and respirators).

5.4. Release

RELEASE OF CHEMICAL AT SITE

The notified chemical will be manufactured and used at the same site. Spillage during manufacture, storage and use is estimated to account for up to 1 kg per annum. These will be contained and collected then disposed of via a licensed solid waste contractor. During manufacture up to 0.2 kg per annum will be released in aqueous effluent, which will be disposed of via a licensed liquid waste contractor. A further 24 kg per annum will be disposed of to the licensed liquid waste contractor in used heptane.

There is a treatment pond on-site which will receive any washings from spills (which will contain only minor amounts of the notified chemical), process reactor cleaning effluent and the effluent from the process area scrubber. It is estimated that up to 2 kg per annum of the notified chemical will be involved.

RELEASE OF CHEMICAL FROM USE

The notified chemical will be used in the manufacture of a polymer product at the same site as manufacture. During polymerisation the notified chemical will be wholly consumed and become irreversibly bound within the polymer product.

The polymer product will be incorporated into a waterborne paint.

5.5. Disposal

In total it is estimated that up to 27.2 kg of the notified chemical will be disposed of annually. The solid wastes containing the notified chemical (1 kg) will go to the licensed landfill managed by the waste contractor. The liquid waste contractor will treat the effluents collected (0.2 kg) or recover the

solvent (24 kg) with any resultant sludge going to landfill or possibly to incineration. The discharge from the on-site treatment pond goes to municipal sewer.

The majority of the notified chemical will share the fate of the paints into which the polymer product, in which the notified chemical is bound, are incorporated. The majority of the paints will be disposed of with the surfaces to which they have been applied which will involve either consignment to landfill or incineration.

5.6. Public exposure

Exposure of the public to the notified chemical is unlikely as it will be site-limited and it will be irreversibly incorporated into the polymer and will not be bioavailable.

6. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa Yellow solid

Melting Point/Freezing Point 77.5 - 78.5°C

METHOD	OECD TG 102 Melting Point/Melting Range.
Remarks	Measured by differential scanning calorimetry (DSC)
TEST FACILITY	Dulux (2005a).

Boiling Point Not determined.

Remarks	Calculated to be 500±24°C using Advanced Chemistry Development (ACD/Labs) Software V8.19.
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Compounds containing similar functional groups are known to undergo thermal degradation at temperatures around 200°C.

Density 1180 kg/m³ at 22°C

METHOD	In house method: A sample of notified chemical was intensely compressed into a hard solid pellet of negligible porosity in a hydraulic press. The dimensions of the disc and its weight were used to calculate the density.
TEST FACILITY	Dulux (2005b).

Vapour Pressure Not conducted

Remarks	Notified chemical is not expected to be volatile.
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Water Solubility <0.5 mg/L (results were below the limits of detection).

METHOD	OECD TG 105 Water Solubility.
Remarks	Flask Method
TEST FACILITY	Leeder Consulting (2005).

Hydrolysis as a Function of pH Not Determined
This test was not conducted because the water solubility of the notified chemical is below the limits of detection (ie <0.5 mg/L). Any test for hydrolysis therefore would not be able to detect changes or the appearance of hydrolysis products. However, there are functional groups present that may hydrolyse at extreme pHs.

Partition Coefficient (n-octanol/water) Not Determined
This test was not conducted because the water solubility of the notified chemical is below the limits of detection (ie

<0.5 mg/L).

A theoretical value of $\log P_{ow} = 7.946 \pm 0.593$ was calculated using ACD Software V8.19 and a calculated value of $\log K_{ow} = 4.59$ was determined using ECOSAR v. 0.99g from the US EPA. Both these values indicate that the neutral species would have a very low affinity for water.

Adsorption/Desorption

Not Determined

This test was not conducted because the water solubility of the notified chemical is below the limits of detection (ie <0.5 mg/L). It is expected that the notified chemical would adsorb to the organic component of soils and sediments and therefore is not expected to be mobile in these media.

Dissociation Constant

Not Determined

This was not determined since it is not soluble in water. The notified chemical contains functional group(s) that have the potential to dissociate weakly in water. The pKa for these groups are typically in the range 2–5. Advanced Chemistry Development (ACD/Labs) Software V8.19 has calculated the pKa as 2.93.

Particle Size

METHOD

Particle size measurement using a Malvern Instruments Mastersizer 2000. A small amount of test substance is dispersed and suspended in water and circulated rapidly through a laser beam. Scattered radiation is detected and analysed to give particle size distribution.

<i>Range (µm)</i>	<i>Volume (%)</i>
<5	0.04
5–50	8.55
50–100	17.38
100–150	16.89
150–200	12.7
200–250	12.56
250–300	5.86
300–400	10.21
400–600	10.47
600–1000	4.98
>1000	0.36

Remarks

Inhalable fraction (fraction ≤ 100 microns) = 26.0%
Respirable fraction (fraction ≤ 10 microns) = 0.6%
Volume weighted mean = 243 µm

TEST FACILITY

Dulux (2005c).

Flash Point

Not conducted

Remarks

Notified chemical is not expected to be volatile

Flammability Limits

Non-flammable, not easily ignitable.

METHOD

Similar to EC Directive 92/69/EEC A.10 Flammability (Solids).

Screening test: A 250 mm long powder train of the sample was placed on a ceramic plate with timing marks at 80 and 180 mm from the start of the sample path. The powder train was ignited at one end using a platinum wire heated to 1000°C. After the first 80 mm of the sample was consumed, the time taken to burn the next 100 mm was measured in seconds.

Remarks	The sample burned briefly (approximately 1 second) with no spread of the fire. The material then proceeded to melt.
TEST FACILITY	Leeder Consulting (2004a).

Autoignition Temperature 275°C

METHOD	Similar to ASTM method G72-01 Standard Test Method for Autogenous Ignition Temperature of Liquids and Solids in a High-Pressure Oxygen-Enriched Environment.
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	The autoignition temperature of the sample was determined using thermal gravimetric analysis (TGA). Three mg of the sample was placed into the TGA under an air atmosphere (5 mL/min). The starting temperature was 100°C and the sample was then heated at 50°C per minute up to a final temperature of 600°C.
Remarks	Complete loss of the sample occurred between 200 and 330°C, with the derivative showing the maximum loss rate at 275°C.
TEST FACILITY	Leeder Consulting (2004b).

Explosive Properties Not determined

Remarks	The flammability test showed that the material is not easily ignitable. In addition, there are no bond groupings present that are known to confer explosive properties.
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Reactivity

Remarks	The chemical does not react with water or air.
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7. TOXICOLOGICAL INVESTIGATIONS

No toxicity data were submitted, however, the applicant has classified the notified chemical as a hazardous substance.

8. ENVIRONMENT

8.1. Environmental fate

No environmental fate data were submitted.

8.2. Ecotoxicological investigations

No ecotoxicity data were submitted.

9. RISK ASSESSMENT

9.1. Environment

9.1.1. Environment – exposure assessment

There will be no direct release of the notified chemical to the aquatic environment. It will be disposed of to landfill via the disposal of spilt material and the sludges generated during effluent treatment by the licensed waste contractor. Some material will be disposed of via the on-site treatment pond and then the municipal sewer.

The US EPA ECOSAR (v3.12) software estimated the adsorption/desorption coefficient K_{oc} to be 1345 and the partition coefficient ($\log K_{ow}$) to be 4.59. These estimates indicate that the notified chemical will not be mobile in soil or sediments and if released to the aquatic environment it will partition to the sediment or suspended organic material. Therefore, in landfill it will adsorb to the soil. In the on-site treatment ponds the notified chemical will

partition out of the water and become associated with the sediment therefore levels in the effluent released to the sewer will be minimal.

The majority of the notified chemical will share the fate of the polymer products, in which it is irreversibly bound, and be disposed of to landfill or incinerated with the cured paints in which the polymer is formulated into.

9.1.2. Environment – effects assessment

No ecotoxicological data was submitted but when modelled using the US EPA ECOSAR (v3.12) software the following results were obtained:

ECOSAR Class	Organism	Endpoint	Predicted concentration (mg/L)
Neutral organic SAR	Fish	14 d LC50	2.612
Esters-acid	Fish	96 h LC50	21.835*
Esters-acid	Daphnid	48 h LC50	12.244*
Esters-acid	Green Algae	96 h EC50	1.912

* Chemical may not be soluble enough to measure predicted effect.

The predicted results indicate that the notified chemical may be toxic to algae. A PNEC using the predicted acute toxicity to green algae (EC50=1.912) and a safety factor of 1000 as only modelled data is available, a PNEC of (1.912/1000) 1.912 µg/L.

The predicted BCF value was 3.162, which indicates that the notified chemical is not likely to bioaccumulate.

9.1.3. Environment – risk characterisation

The majority of the notified chemical will be disposed of bound within an inert polymer matrix of paints and not be released to the aquatic environment. Since the notified chemical will not be released to the aquatic environment the risk associated with the manufacture and proposed use is likely to be low.

9.2. Human health

9.2.1. Occupational health and safety – exposure assessment

Dermal, inhalation and ocular exposure to airborne dust particles of the notified chemical may occur during sampling, analysis, packaging, reactor cleaning and maintenance. In addition, dermal, inhalation and ocular exposure to the notified chemical may also occur when it is added as a raw material in the manufacture of the polymer into which the notified chemical (<20%) is incorporated. Exposure should be minimised by the use of engineering controls such as local exhaust ventilation, and the use of personal protective equipment by workers.

9.2.2. Public health – exposure assessment

The exposure of the public to the notified chemical during its manufacture and the manufacture of the final polymer into which it is incorporated is expected to be negligible.

9.2.3. Human health – effects assessment

No toxicological data have been provided for the notified chemical and therefore the substance cannot be classified in accordance with the NOHSC *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

The notified chemical contains a high concern functional group, which is structurally related to a functional group that has a structural alert for sensitisation (Barratt, 1994). In addition, high dermal absorption is expected (up to 100%), based upon the molecular weight of the notified chemical (MW<500), and its predicted partition coefficient (logPow>4) (European Commission, 2003). Therefore, there is the potential for skin sensitisation to occur upon exposure to the notified chemical.

The notified chemical may undergo degradation to form carbon disulfide. Carbon disulfide is classified by the following health risk phrases (HSIS, 2006):

R62 Possible risk of impaired fertility
R63 Possible risk of harm to the unborn child
R48/23 Danger of serious damage to health by prolonged exposure through inhalation
R36/38 Irritating to eyes and skin

9.2.4. Occupational health and safety – risk characterisation

The notified chemical has not been tested for any toxicological properties but may be a skin sensitiser based on the presence of a high concern functional group, molecular weight and partition coefficient. Irritation and adverse effects resulting from inhalation of the notified chemical are also possible. Given that exposure of workers to the notified chemical during manufacture and end use is mitigated through the use of engineering controls and personal protective equipment, the occupational health and safety risk of the notified chemical is considered to be low.

The notified chemical has approximately 26% with a particle size <100µm (inhalable fraction) and 0.6% with <10µm (respirable fraction). Given the low water solubility of the notified chemical, any dust that deposits in the nasopharyngeal region (>1-5 µm) could be coughed or sneezed out of the body, or swallowed. Dust depositing in the tracheobronchial region (<1-5 µm) would be mainly cleared from the lungs and swallowed (European Commission, 2003). This will occur to only a small fraction of the dust. However, irritant or toxic effects as a result of inhalation of the notified chemical can not be ruled out.

The notified chemical has the potential to degrade to carbon disulfide, particularly at elevated temperatures (approximately 200°C). This is unlikely to occur during manufacture and handling of the notified chemical (~25-30°C), when cleaning the reactor with boiling water, or during the polymerisation (~85-90°C). If carbon disulfide were to be formed, workers may be exposed by inhalation of the vapours or by contact with the skin or eyes. However, levels are unlikely to exceed the current exposure standard for carbon disulfide (10ppm TWA). Carbon disulfide would also present a fire hazard due to its volatility, low autoignition point, and high flammability. The engineering controls and personal protective equipment used at the manufacture site should mitigate the occupational health and safety risk associated with the possible presence of carbon disulfide.

9.2.5. Public health – risk characterisation

The exposure of the public to the notified chemical is expected to be negligible; therefore the risk to public health is negligible.

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

10.1. Hazard classification

No toxicological data have been provided for the notified chemical and therefore the substance cannot be classified in accordance with the NOHSC *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004).

and

Classification of the notified chemical using the Globally Harmonised System for the Classification and Labelling of Chemicals (GHS) (United Nations 2003) cannot be undertaken as no toxicological or ecotoxicological data were available. This system is not mandated in Australia and carries no legal status but is presented for information purposes.

10.2. Environmental risk assessment

The chemical is not considered to pose a risk to the environment based on its reported use pattern.

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 in the proposed manner.

11. MATERIAL SAFETY DATA SHEET

11.1. Material Safety Data Sheet

The MSDS of the notified chemical provided by the notifier was assessed in accordance with the NOHSC *National Code of Practice for the Preparation of Material Safety Data Sheets* (NOHSC 2003). 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 1994). The accuracy of the information on the label remains the responsibility of the applicant.

12. RECOMMENDATIONS

CONTROL MEASURES

Occupational Health and Safety

- Employers should implement the following engineering controls to minimise occupational exposure to the notified chemical:
 - Local exhaust ventilation during all operations involving the notified chemical.
- Employers should implement the following safe work practices to minimise occupational exposure during handling of the notified chemical:
 - Avoid generating and breathing dust.
 - Avoid skin and eye contact.
 - Restricted access to the work area.
- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemical:
 - Elbow-length impervious gloves
 - Protective clothing such as overalls
 - Full face shield and respirator

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 the notifier to minimise environmental exposure during manufacture and use of the notified chemical:
 - All process and storage areas should be bunded with any drains present going to the on-site treatment system.

Disposal

- The notified chemical should be disposed of by licensed waste contractors.

Storage

- The following precautions should be taken regarding storage of the notified chemical:
 - Store away from sources of heat or ignition.
 - Store away from amines, bases and oxidising agents.

Emergency procedures

- Spills or accidental release of the notified chemical should be handled by containment, collection by an appropriate absorbent material, then placed in labelled containers ready for disposal via a licensed waste contractor.

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 importation volume exceeds ten tonnes per annum notified chemical
 - the notified chemical will not be site-limited

or

- (2) Under Section 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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