

April 2011

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

**FULL PUBLIC REPORT**

**LTD/1515: Zirconium organometallic complex 1 in BMC-200-AI  
LTD/1516: Zirconium organometallic complex 2 in BMC-200-AI**

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

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

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  
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**FULL PUBLIC REPORT****LTD/1515: Zirconium organometallic complex 1 in BMC-200-AI**  
**LTD/1516: Zirconium organometallic complex 2 in BMC-200-AI****1. APPLICANT AND NOTIFICATION DETAILS**

## APPLICANT(S)

Qenos Pty Ltd (ABN: 62 054 196 771)  
231-238 Maidstone Street  
Altona, VIC 3018

## NOTIFICATION CATEGORY

LTD/1515: Limited-small volume: Chemical other than polymer (1 tonne or less per year).

LTD/1516: Limited-small volume (reduced fee notification): Chemical other than polymer (1 tonne or less per year). Chemical is being notified at the same time as a chemical which is similar.

## EXEMPT INFORMATION (SECTION 75 OF THE ACT)

Data items and details claimed exempt from publication: chemical name, other names, CAS number, molecular and structural formulae, molecular weight, analytical data, degree of purity, impurities, additives/adjuvants, use details and import volume.

## VARIATION OF DATA REQUIREMENTS (SECTION 24 OF THE ACT)

Variation to the schedule of data requirements is claimed as follows: all physico-chemical endpoints.

## PREVIOUS NOTIFICATION IN AUSTRALIA BY APPLICANT(S)

None

## NOTIFICATION IN OTHER COUNTRIES

None

**2. IDENTITY OF CHEMICAL**

## MARKETING NAME(S)

PRODIGY(TM) Bimodal Catalyst BMC-200-X4 (<10% of each of the notified chemicals)  
PRODIGY(TM) BMC-200-X4 Bimodal Catalyst  
PRODIGY(TM) Bimodal Catalyst BMC-200  
PRODIGY(TM) BMC-200 Bimodal Catalyst

## MOLECULAR WEIGHT

>500 Da

**3. COMPOSITION**

DEGREE OF PURITY      Inseparable reaction mixture

**4. PHYSICAL AND CHEMICAL PROPERTIES**

APPEARANCE AT 20°C AND 101.3 kPa: The imported product is a yellow-to-brown suspension of the notified chemicals on silica in hydrocarbon solvent. When settled, the powder appears as a mud layer at the bottom of the container. The notified chemicals are not isolated from this mixture.

Property	Value	Data Source/Justification
Melting Point/Freezing Point	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Boiling Point	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Density	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.

Viscosity	200-800 cP at 25 °C	Determined for the imported product using a Brookfield viscometer. Study report was not provided.
Vapour Pressure	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Water Solubility	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Hydrolysis as a Function of pH	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Partition Coefficient (n-octanol/water)	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Adsorption/Desorption	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Dissociation Constant	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Particle Size	Average = 24 micron	Determined for the imported product using light scattering. Study report was not provided.
Flash Point	6.75 °C at 101.3 kPa	Determined for the imported product.
Flammability	Pyrophoric	The notified chemicals will spontaneously ignite when exposed to air.
Autoignition Temperature	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Explosive Properties	Not determined	Chemicals not isolated and high reactivity precludes study from being conducted.
Stability Testing	Thermally stable to >200 °C	Determined for the powdered reaction mixture under a nitrogen atmosphere, using differential scanning calorimetry.

#### DISCUSSION OF PROPERTIES

##### *Reactivity*

The notified chemicals are catalyst components that are pyrophoric and highly reactive with water/alcohols. They will degrade upon reaction with air, water and during end-use.

##### *Dangerous Goods classification*

Based on the submitted physical-chemical data in the above table the notified chemicals are classified as follows according to the Australian Dangerous Goods Code (NTC, 2007).

Class 4.2 – Substances liable to spontaneous combustion (Packing Group 1)

The data above do not address all Dangerous Goods endpoints. Therefore, consideration of all endpoints should be undertaken before a final decision on the Dangerous Goods classification is made by the introducer of the chemicals.

## 5. INTRODUCTION AND USE INFORMATION

#### MODE OF INTRODUCTION OF NOTIFIED CHEMICAL (100%) OVER NEXT 5 YEARS

The notified chemicals will be imported as a solvent solution at <10% concentration.

#### 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>
LTD/1515	<i>Tonnes</i>	≤1	≤1	≤1	≤1	≤1
LTD/1516	<i>Tonnes</i>	≤1	≤1	≤1	≤1	≤1

#### PORT OF ENTRY

Melbourne

#### IDENTITY OF MANUFACTURER/RECIPIENTS

Qenos Australia Pty Ltd

**TRANSPORTATION AND PACKAGING**

The notified chemicals (at <10% concentration) will be supplied in 119 gallon metal containers and transported to the recipient by road. The notified chemicals will be stored in the original unopened containers under an inert atmosphere.

**USE**

The notified chemicals will be used as components of a catalyst system for polyethylene production.

**OPERATION DESCRIPTION**

Upon delivery of the notified chemicals (at <10% concentration) to polyethylene production sites, they will be transferred, via a strainer (to remove agglomerated material), to a feed vessel, using closed system transfer and nitrogen pressure. They will then be pumped into the polymerization reactor. The notified chemicals will be encapsulated into the polyethylene and will be removed from the reactor as part of the polyethylene. The product polyethylene will be transferred to a storage bin for packaging and shipment.

Due to the reactive nature of the notified chemicals, closed system transfers will be necessary. Prior to line disconnection, the system will be flushed and the residue collected as hazardous waste. As necessary, the catalyst strainer is removed from its housing and the contents emptied into a hazardous waste collection container. Emptied product containers will be returned to the international supplier for cleaning.

The polyethylene production unit will be contained in an outdoor environment, i.e. in an unconfined area that is subject to outside ambient conditions and open to the atmosphere.

**6. HUMAN HEALTH IMPLICATIONS****6.1. Exposure Assessment****6.1.1. Occupational Exposure****NUMBER AND CATEGORY OF WORKERS**

<i>Category of Worker</i>	<i>Number</i>	<i>Exposure Duration (hours/day)</i>	<i>Exposure Frequency (days/year)</i>
Transport Worker (transfer from storage to process areas)	1	Unspecified	~70
Operator (Connection/disconnection of lines)	1	0.25	~70
Operator (Cleaning strainer in feed line)	1	1	~180
Maintenance (pump maintenance)	1	1	~12
Operator (disconnection and transport of waste collection container)	1	1	~12

**EXPOSURE DETAILS**

Transport and storage workers are unlikely to be exposed to the notified chemicals (at <10% concentration) except in the event of an accident.

Due to the closed-system operation at the polyethylene production site, exposure of workers to the notified chemicals is expected to be minimal. Dermal or ocular exposure to the notified chemicals may occur whilst connecting and disconnecting transfer lines, whilst emptying/cleaning the strainer and during pump maintenance. However, exposure should be mitigated through the flushing of the system prior to hose disconnection and through the use of personal protective equipment (PPE: goggles, impervious gloves, protective clothing).

**6.1.2. Public Exposure**

The notified chemicals are intended for industrial use only, therefore the public may be exposed to the notified chemicals (at <10% concentration) only in the event of a transport accident. The public may come into contact with the manufactured polyethylene. However, as the notified chemicals will have reacted and become encapsulated into the polyethylene, they will be unavailable for exposure.

**6.2. Human Health Effects Assessment**

No toxicity data were submitted. The generation of such data is precluded by the high reactivity of the notified chemicals.

The notified chemicals will spontaneously ignite when exposed to air. Therefore, any exposure is expected to be to the degradation products, including metal oxides and hydroxides and oxides of carbon.

Based on the expected negligible lipophilicity of the inorganic degradation products of the notified chemicals, passive diffusion across the gastrointestinal (GI) tract and dermal absorption is unlikely to occur.

The degradation products do not contain any structural alerts for toxic effects. The results of studies conducted on the inorganic degradation products suggest that the chemicals are of low acute oral toxicity in rats (LD50 >5000 mg/kg bw), non-irritating to the skin and eyes of rabbits and non-mutagenic to bacteria (IUCLID, 2000a and IUCLID, 2000b).

The notifier has classified the notified chemicals as sensitisers.

#### **Health hazard classification**

In the absence of toxicity data, the notified chemicals cannot be classified according to the *Approved Criteria for Classifying Hazardous Substances* (NOHSC, 2004). However, the notifier has classified the chemicals with the following risk phrase:

R43 May cause sensitisation by skin contact

### **6.3. Human Health Risk Characterisation**

#### **6.3.1. Occupational Health and Safety**

The notified chemicals will be handled by workers at <10% concentration. The notified chemicals themselves are classified as a Class 4.2 Dangerous Good according to the Australian Dangerous Goods Code (NTC, 2007), i.e. they are liable to spontaneous combustion. Transport, storage and handling of products containing the notified chemicals in accordance with the above code and the *NOHSC National Code of Practice for the Storage and Handling of Workplace dangerous Goods* (NOHSC, 2001) should minimise the risk involved for transport and storage workers.

The primary risks associated with use of the notified chemicals will be due to the abovementioned high reactivity. While the reactivity of the chemicals preclude toxicological studies from being conducted, the potential for sensitisation following skin contact cannot be excluded. However, given the high reactivity, exposure to the notified chemicals themselves is expected to be minimal.

Due to the reactive nature of the chemicals, closed-system operations will be necessary. Therefore, provided that control measures are in place to minimise worker exposure, including the use of enclosed/automated processes and PPE, and transport, storage and handling are in accordance with the Dangerous Goods Codes, the risk to the health of workers from use of the notified chemicals is not considered to be unacceptable.

#### **6.3.2. Public Health**

The notified chemicals are intended for use in industrial settings by trained workers. The public may be exposed to the manufactured polyethylene. However, the notified chemicals will have reacted and become encapsulated into the polyethylene and will be unavailable for exposure. Therefore, when used in the proposed manner, the risk to public health from the notified chemicals is not considered to be unacceptable.

## **7. ENVIRONMENTAL IMPLICATIONS**

### **7.1. Environmental Exposure & Fate Assessment**

#### **7.1.1. Environmental Exposure**

##### **RELEASE OF CHEMICAL AT SITE**

The notified chemicals will be imported into Australia as components of a finished product in pressure rated metal containers. Accidental spills and leaks during transport are unlikely. However, in the case of an accidental release the notified chemicals are expected to be disposed of by a licensed waste contractor.

##### **RELEASE OF CHEMICAL FROM USE**

Empty containers containing residues of the notified chemicals will be exported to be cleaned, refurbished and reused. Due to their reactive nature and use in a closed system, release of the notified chemicals to the environment during use is expected to be negligible. Agglomerated product, line flushes and drainings containing the residues of the notified chemicals will be collected and disposed of by a licensed waste contractor. The majority of imported notified chemicals will be consumed during the polymerisation process and encapsulated in the manufactured polyethylene.

##### **RELEASE OF CHEMICAL FROM DISPOSAL**

The reacted notified chemicals will share the fate of the polyethylene in which they are encapsulated and are expected to be disposed of to landfill.

#### **7.1.2. Environmental Fate**

No environmental fate data were submitted. Aquatic exposure to the notified chemicals is not expected when they are used as proposed in the industrial manufacture of polyethylene. However, if the notified chemicals are released to the aquatic environment they will rapidly react to form water, refractory insoluble metal oxides and hydroxides, oxides of carbon and nitrogen and inorganic salts. In landfill, the notified chemicals will have reacted and be encapsulated in polyethylene and therefore will not be exposed to the environment. The reacted notified chemicals in the polyethylene articles are not likely to be bioavailable nor bioaccumulative and are expected to decompose to form the same products as formed on contact with water.

#### **7.1.3. Predicted Environmental Concentration (PEC)**

A PEC was not determined because very little of the notified chemicals is expected to be released to the aquatic compartment when the chemicals are used as proposed in the manufacture of polyethylene. Moreover, the notified chemicals are not expected to persist in water due to their reactivity.

### **7.2. Environmental Effects Assessment**

No ecotoxicity data for the notified chemicals were submitted. On contact with air or water the notified chemicals will rapidly react to form refractory insoluble metal oxides and hydroxides which will therefore be neither bioavailable nor bioaccumulative.

#### **7.2.1. Predicted No-Effect Concentration (PNEC)**

The PNEC was not calculated as no ecotoxicity data are available for the notified chemicals and there is expected to be very little exposure of the notified chemicals to the water compartment based on the proposed use pattern.

### **7.3. Environmental Risk Assessment**

All spillages and waste containing the notified chemicals are expected to be disposed to by licensed waste contractors according to State/Territory regulations. During use, the majority of the notified chemicals will be consumed during the polymerisation process and immobilised within a cured inert polymerised polyethylene matrix rendering them unavailable to the environment. On contact with air or water the notified chemicals will rapidly react to form refractory insoluble metal oxides and hydroxides and non-metal oxides. The notified chemicals' reaction products will therefore be neither bioavailable nor bioaccumulative. Since there is expected to be very limited exposure to aquatic organisms, the notified chemicals are therefore not expected to pose an unacceptable risk to the environment based on their proposed use pattern.

## 8. CONCLUSIONS AND REGULATORY OBLIGATIONS

### Hazard classification

In the absence of toxicity data, the notified chemicals cannot be classified according to the *Approved Criteria for Classifying Hazardous Substances* [NOHSC:1008(2004)]. However, the notifier has classified the chemicals with the following risk phrase:

R43 May cause sensitisation by skin contact

### Human health risk assessment

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

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

### Environmental risk assessment

On the basis of the reported use pattern, the notified chemicals are not considered to pose an unacceptable risk to the environment.

### Recommendations

#### REGULATORY CONTROLS

##### Hazard Classification and Labelling

- The notified chemicals should be classified as follows under the ADG Code:
  - Class 4.2 – Substances liable to spontaneous combustion (Packing Group 1)
- As the notified chemicals are dangerous goods, the applicant should ensure that the MSDS and labels for products containing the notified chemicals are acceptable to the relevant state authority.

#### CONTROL MEASURES

##### Occupational Health and Safety

- Employers should implement the following engineering controls to minimise occupational exposure to the notified chemicals as introduced (<10%):
  - Enclosed, automated processes
  - Use under an inert atmosphere
- Employers should implement the following safe work practices to minimise occupational exposure during handling of the notified chemicals as introduced (<10%):
  - Avoid contact with skin and eyes
  - Avoid spills and splashing during use
  - Prevent leaks and spills
- Employers should ensure that the following personal protective equipment is used by workers to minimise occupational exposure to the notified chemicals as introduced (<10%):
  - Coveralls, gloves, goggles

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 chemicals 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 chemicals should be disposed of to landfill.

### Storage

- The following precautions should be taken by storage managers regarding storage of the notified chemicals as introduced:
  - Store in original unopened container under an inert atmosphere.
  - The handling and storage of the notified chemicals should be in accordance with the *NOHSC National Code of Practice for the Storage and Handling of Workplace dangerous Goods* [NOHSC:2017(2001)] or relevant State or Territory regulations.

### Emergency procedures

- Spills or accidental release of the notified chemicals should be handled by physical containment, collection and subsequent safe disposal.
- In the event of an emergency, unnecessary personnel should be evacuated and all ignition sources removed.

### Transport and Packaging

- The transportation of the notified chemicals should be in accordance with the *Australian Code for the Transport of Dangerous Goods by Road and Rail (ADG code)* (NTC, 2007).

## 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 chemicals 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 chemicals, have post-assessment regulatory obligations to notify NICNAS when any of these circumstances change. These obligations apply even when the notified chemicals are listed on the Australian Inventory of Chemical Substances (AICS).

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

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

or

- (2) Under Section 64(2) of the Act; if
  - the function or use of the chemicals has changed from catalysts for polyethylene production, or is likely to change significantly;
  - the chemicals have begun to be manufactured in Australia;
  - additional information has become available to the person as to adverse effects of the chemicals on occupational health and safety, public health, or the environment.

The Director will then decide whether a reassessment (i.e. a secondary notification and assessment) is required.

*Material Safety Data Sheet*

The MSDS of a product containing the notified chemicals provided by the notifier was reviewed by NICNAS. The accuracy of the information on the MSDS remains the responsibility of the applicant.

### **BIBLIOGRAPHY**

- Chilworth (2008) Determination of Flash Point Temperature (Reference number: AK/8079/0808/AK, August, 2008), Plainsboro, U.S.A, Chilworth Technology Inc. (Unpublished report submitted by the notifier).
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- NTC (National Transport Commission) 2007 Australian Code for the Transport of Dangerous Goods by Road and Rail (ADG code), 7th Edition, Commonwealth of Australia.