Australian Government
Department of Health
Australian Industrial Chemicals Introduction Scheme

1*H*-1,4,7-Triazonine, octahydro-1,4,7-trimethyl-

Assessment statement

1 April 2022

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AICIS assessment statement

Chemical in this assessment

Name	CAS registry number
1*H*-1,4,7-Triazonine, octahydro-1,4,7-trimethyl-	96556-05-7

Reason for the assessment

An application to vary the terms of an Inventory listing under section 88 of *the Industrial Chemicals Act 2019* (the Act).

The chemical has been previously assessed (LTD/1898) and is listed on the Australian Inventory of Industrial Chemicals (the Inventory). An introducer applied to vary the specific requirements to provide information (see **supporting information**) to increase the introduction volume (up to 10 tonnes) and the introduction concentration (up to 3% for reformulation in Australia).

Defined scope of assessment

The chemical has been assessed to determine whether the risks to human health and the environment associated with the proposed variation to the specific requirements to provided information can be managed.

Summary of assessment

Summary of introduction, use and end use

The assessed chemical will be imported into Australia as a component of a formulation at up to 3% concentration for local reformulation into paints and coatings. Based on the information submitted for this application, the imported formulation for local reformulation will contain a counter acid, resulting in a pH value of 8. However, as the chemical is listed on the Inventory, various formulations at various pH values may be introduced into Australia for local reformulation. The assessed chemical will also be imported as a component in end use paints and coatings at up to 0.3% concentration. End use products containing the assessed chemical at up to 0.3% concentration will be used by professionals and do-it-yourself (DIY) consumers.

Physical hazard classification

Based on the available physico-chemical data (see **supporting information**), the assessed chemical satisfies the criteria for physical hazard classification according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS, United Nations 2017), as adopted for industrial chemicals in Australia.

Physical hazard	Hazard category	Hazard statement
Flammable liquids	Flam. Liquid 4	H227: Combustible liquid

Human health

Summary of health hazards

No additional toxicological data were provided for the assessed chemical in this application. Based on the pH data provided for LTD/1898 (NICNAS, 2016), the assessed chemical is likely to be corrosive warranting hazard classification. However, some formulations imported at up to 3% concentration for local reformulation may contain other ingredients such as a counter acid to remove or reduce corrosive properties by reducing the pH value of the formulation (such as the imported formulation assessed under this variation application). In end use products containing the chemical at up to 0.3% concentration, the pH value is expected to be significantly reduced and therefore the potential for causing corrosive effects to end uers is not expected (see **supporting information**).

Health hazard classification

Based on the available data, the assessed chemical satisfies the criteria for classification for human health according to the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS, United Nations 2017), as adopted for industrial chemicals in Australia.

Health hazards	Hazard category	Hazard statement
Corrosion/irritation	Skin Corr. 1	H314: Causes severe skin burns and eye damage

Summary of health risk

Public

When introduced and used in the proposed manner, the public will be exposed to the chemical:

- at concentrations up to 0.3%
- by incidental skin and eye contact with the chemical during use of paint and coatings.

Based on the available hazard information the chemical has low toxicity at exposed concentrations. Although effects from prolonged exposure cannot be ruled out the frequency and extent of exposure is expected to be less than that of professional workers. Therefore, there are no identified risks to the public that require specific risk management measures, if the assessed chemical is introduced and used in accordance with the terms of the Inventory listing.

Workers

Workers may be exposed to the assessed chemical at up to 3% concentration during reformulation of paints and coatings.

Although dermal, ocular and inhalation exposure to the assessed chemical (at up to 0.3% concentration) could occur during application of the paint, based on the available hazard information the chemical has low toxicity at these concentrations although effects from repeated exposure cannot be ruled out.

Given the critical local health effects, the chemical could pose a risk to workers. Control measures to minimise dermal,ocular and inhalation exposure are needed to manage the risk to workers (refer to **means for managing risks** section).

Environment

Summary of environmental hazard characteristics

According to domestic environmental hazard thresholds and based on the available data the chemical is:

- Persistent (p)
- Not bioaccumulative (not b)
- Not toxic (not t)

Environmental hazard classification

Based on the ecotoxicological information available for the assessed chemical, it does not exceed the toxicity thresholds to be harmful to aquatic life. Therefore, the assessed chemical does not satisfy the criteria for classificatiion under the *Globally Harmonised System of Classification and Labelling of Chemicals* (GHS, United Nations 2017) for acute and chronic aquatic toxicities.

Summary of environmental risk

The assessed chemical will be introduced as an additive for use in paints and coatings. This use may result in the release of the assessed chemical to sewers and surface waters. In these compartments, the assessed chemical is expected to adsorb to soils, sediments or sewage treatment plant (STP) sludge.

The assessed chemical is not readily degradable. The assessed chemical has a low potential for bioaccumulation and is not toxic to aquatic organisms.

As the assessed chemical is not PBT it is unlikely to have unpredictable long-term effects and its risk may be estimated by the risk quotient method (RQ = PEC ÷ PNEC). Based on the RQ < 1, the assessed chemical is unlikely to cause environmental risks.

Means for managing risks

Inventory listing

Following the finalisation of this assessment, the specific requirements to provide information (see **supporting information**) are varied as follows:

The Executive Director must be notified in writing within 28 days if:

1. the importation volume of the chemical exceeds ten tonnes per annum;

2. the concentration of the chemical exceeds or is intended to exceed 0.3% in paints or coatings.

If, since the chemical was assessed under the *Industrial Chemicals (Notification and Assessment) Act 1989*, a person who introduces the chemical becomes aware that–

a) the function or use of the chemical has changed, or is likely to change, significantly, subject to the following exception:
   i. the chemical is introduced at a concentration of up to 3% for use in the formulation of paint; or
b) the amount of the chemical being introduced has increased, or is likely to increase, significantly; or
c) in the case of a chemical not manufactured, or proposed to be manufactured, in Australia at the time of the assessment – it has begun to be manufactured in Australia; or
d) the method of manufacture of the chemical in Australia has changed, or is likely to change, in a way that may result in an increased risk of an adverse effect of the chemical on occupational health and safety, public health or the environment; or
e) 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 person must, within 28 days of becoming aware, notify the Executive Director in writing of the circumstances of which they have become aware.

Workers

Information relating to safe introduction and use

- The information in this statement, including hazard classifications, should be used by a person conducting a business or undertaking (PCBU) at a workplace (such as an employer) to determine the appropriate controls under the relevant jurisdiction Work Health and Safety laws.

- The following control measures could be implemented to manage the risk arising from exposure to the assessed chemical during reformulation:

  - Use of engineering controls such as
    - Enclosed, automated processes where possible
    - Local exhaust ventilation

  - Use of safe work practices to
    - Avoid contact with skin and eyes
    - Avoid inhalation of aerosols or mists

  - Using personal protective equipment (PPE) that is designed, constructed and operated to ensure that the worker does not come into contact with the chemical including:
    - Protective clothing
    - Impervious gloves
    - Safety glasses
    - Respiratory protection if inhalation exposure may occur

- The following control measures could be implemented to manage the risk arising from exposure to the assessed chemical during end use activities:
    - Use of engineering controls such as
        - Spray booths during spray applications where possible
    - Use of safe work practices to
        - Avoid contact with skin and eyes
        - Avoid inhalation of aerosols or mists
- Spray applications of the assessed chemical should be carried out in accordance with the Safe Work Australia Code of Practice for Spray Painting and Powder Coating (SWA, 2020) or relevant State or Territory Code of Practice.
- The storage of the assessed chemical as introduced for reformulation should be in accordance with the Safe Work Australia Model Code of Practice for Managing Risks of Hazardous Chemicals in the Workplace (SWA, 2021) or relevant State or Territory Code of Practice.
- A copy of the SDS should be easily accessible to reformulation workers.

Environment

No specific recommendations for safe use of the assessed chemical are required when the assessed chemical is introduced in accordance with the terms of the Inventory listing.

Conclusions

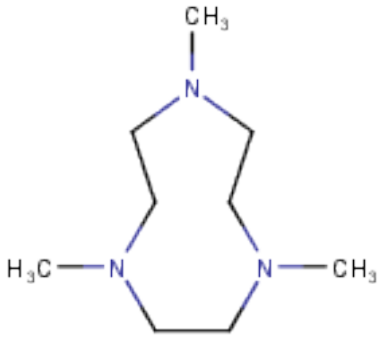
The conclusions of this assessment are based on the information described in this statement.

Considering the proposed means of managing risks, the Executive Director is satisfied that the human health and environment risks associated with the variation of the terms of the Inventory listing can be managed within existing risk management frameworks. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory and the proposed means of managing the risks identified during this assessment are implemented.

Note: Obligations to report additional information about hazards under section 100 of the *Industrial Chemicals Act 2019* (the Act) apply.

Supporting information

Chemical identity

Chemical name	1*H*-1,4,7-Triazonine, octahydro-1,4,7-trimethyl-
CAS No.	96556-05-7
Synonyms	Dragon Ligand (trade name) 1,4,7-Trimethyl-1,4,7-triazacyclononane Me3TACN MeTACN
Structural formula	
Molecular formula	$C_9H_{21}N_3$
Molecular weight (g/mol)	171.28
SMILES	N1(C)CCN(C)CCN(C)CC1
Chemical Description	The assessed chemical has a degree of purity greater than 95%.

Relevant physical and chemical properties

Physical form	Pale yellow liquid
Melting point	< -20 °C
Boiling point	207.3 °C at 101.4 kPa
Density	989 kg/m^3 at 20 °C
Vapour pressure	0.123 kPa at 25 °C
Water solubility	> 50 g/L at 20 °C
Henry's law constant	2.06 x 10^{-7} Pa.m^3/mol (calc.)
Ionisable in the environment?	Yes

pKa	8.63, 5.75, 2.86 (base; calc.)
log K_{ow}	0.446 at pH 7
Flash point	69 °C at 100.9 kPa
Autoignition Temperature	200 °C

Introduction and use

The assessed chemical will be imported into Australia either as a component of a formulation at up to 3% concentration for reformulation of end use paints and coatings or as a component in end use paints and coatings at up to 0.3% concentration.

The assessed chemical will be imported and distributed in containers of varying sizes ranging from 5 L steel drums, up to 20 L polypropylene or metal cans (tin plate) to 200 L steel drums. The containers will be transported to the warehouse or to the reformulation site by road. Reformulation processes are likely to be highly automated and use closed systems with adequate waste management and ventilation systems in place, in accordance with individual state and territory regulations. Finished consumer products containing the assessed chemical at up to 0.3% concentration will be packaged in containers suitable for retail sale.

End use products will be applied by brush, roller or spray onto a wide range of substrates by both professionals and DIY users.

Existing Australian regulatory controls

AICIS

The chemical is listed on the Inventory with specific requirements to provide information as a term of the inventory listing. This term is published as:

- Specific information requirement: Obligations to provide information apply. You must tell us within 28 days if the circumstances of your importation or manufacture (introduction) are different to those in our assessment

Under *Section 75(2)(c) of the Industrial Chemicals (Consequential Amendments and Transitional Provisions) Rules 2019* the notification obligations under *Subsections 64(1) and (2) of the old law (ICNA Act)* are taken to be specific information requirements to be provided to the Executive Director.

The assessment report recommended the following circumstances under which the Director must be notified, by an introducer in writing, within 28 days (*Section 64(1) of* the *Industrial Chemicals Notification and Assessment (ICNA) Act 1989*)

- the importation volume exceeds one tonne per annum of the chemical;
- the concentration of the chemical exceeds or is intended to exceed 0.3% in paints or coatings;

Additionally under Section 64(2) of the ICNA Act, a person who introduces an industrial chemical that has been assessed under this Act must within 28 days of becoming aware of any of the following circumstances since the assessment, notify the Director in writing:

- the function or use of the chemical has changed, or is likely to change, significantly;
- the amount of the chemical being introduced has increased, or is likely to increase, significantly;
- in the case of a chemical not manufactured, or proposed to be manufactured, in Australia at the time of the assessment - it has begun to be manufactured in Australia
- the method of manufacture of the chemical in Australia has changed, or is likely to change, in a way that may result in an increased risk of an adverse effect of the chemical on occupational health and safety, public health or the environment
- 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;

Human exposure

Workers

Reformulation

Typically, reformulation processes may incorporate blending operations that are highly automated and occur in a fully enclosed/contained environment, followed by automated filling using sealed delivery systems into containers of various sizes. Dermal, ocular and inhalation exposure (if aerosols or mists are formed) of workers to the assessed chemical at up to 3% concentration may occur during manual transfer, quality control analysis, and cleaning and maintenance of equipment. Exposure is expected to be minimised through the use of enclosed and automated systems, local exhaust ventilation and PPE for workers including protective clothing, impervious gloves, safety glasses and appropriate respiratory protection if inhalation exposure may occur.

Professional End Use

Dermal, ocular and inhalation (if aerosols or mists are formed) exposure to the assessed chemical (at up to 0.3% concentration) may occur during manual transfer of the paint or coating to application equipment, during application (by brush, roller or spray) and also during equipment cleaning and maintenance. Exposure is expected to be minimised by avoiding contact with skin and eyes and inhalation of aerosols or mists. Once the paint or coating is cured and dried, the assessed chemical will be bound within the solid matrix and will not be available for exposure.

Public

Paints and coatings containing the assessed chemical (at up to 0.3% concentration) will be available for use by DIY users. Exposure (dermal, ocular and inhalation) is expected to be on a less frequent basis than for professional end users, although PPE may not be worn.

The public may come into contact with substrates coated with paints or coatings containing the assessed chemical. However, once the paint or coating is cured and dried, the assessed chemical will be bound within the solid matrix and will not be available for exposure.

Health hazard information

No toxicological data for the assessed chemical were provided.

Toxicokinetics

The assessed chemical has a low molecular weight (171.28 g/mol) and a log kow of 0.446. Therefore, absorption across biological membranes is expected. However the high water solubility of the assessed chemical (> 50 g/L at 20 °C) may limit dermal absorption.

Corrosion/Irritation

Based on the data provided for LTD/1898 (NICNAS, 2016), the pH of an aqueous solution containing 1% assessed chemical was measured to be 12.53 and hence the assessed chemical is classified as skin corrosion/irritation (Category 1): H314 - causes severe skin burns and eye damage according to GHS criteria as adopted in Australia for industrial chemicals. However, some formulations imported at up to 3% concentration for local reformulation may contain other ingredients that can reduce and eliminate corrosive effects by changing the pH value. For example, the formulation to be introduced under this variation application will contain a counter acid, resulting in a pH value of 8. The potential for causing corrosive effects is not expected in end use paints and coatings containing the chemical at up to 0.3% concentration. The assessed chemical is expected to form a complex with a metal salt in the product to significantly reduce the pH value. In addition, other components of the paint or coating are expected to act as a buffer further reducing the pH value of the product.

Environmental exposure

The assessed chemical will be imported into Australia in paint/coating additive products for reformulation (containing up to 3% assessed chemical) or in end use paints and coatings (containing up to 0.3% assessed chemical). There is unlikely to be any significant release to the environment from transport and storage of these products, except in the case of accidental spills and leaks.

Reformulation processes involving the assessed chemical are expected to involve manual dispensing of the chemical into a closed mixing vessel. The finished paint and coating will then be sealed in cans prior to use by end users. Any accidental spills, leaks, or waste containing the assessed chemical generated during these processes are expected to be collected and disposed according to local government regulations.

Products containing the assessed chemical will be used by both professionals and DIY users. During applications, paints and coatings containing the assessed chemical are expected to be applied by brush, roller and spray techniques. Some overspray will occur during spray application, but this technique is expected to be performed primarily by professional workers with processes in place to minimise release of the assessed chemical.

During applications, the assessed chemical may also be released to the environment as accidental spills and container residues. It is estimated that up to 3% may be released from accidental spills during use or be present in container residues. These releases are expected to be collected and disposed in accordance with local government regulations.

When the products containing the assessed chemical have cured, the assessed chemical is expected to be chemically bound into the solid matrix. As such, it will share the fate of the

substrate to which it has been applied, and is predominantly expected to be disposed to landfill, or thermally decomposed during metal reclamation.

Residues containing the assessed chemical on brushes and rollers are expected to be rinsed into containers and then collected and disposed of appropriately. While it is expected that professional workers will correctly dispose of any coatings waste, DIY users of paints and coatings may be more likely to incorrectly rinse residues “down the drain”. As a worst-case scenario, it is assumed that up to 5% of the introduced assessed chemical may be incorrectly disposed of to the sewer, drains, or ground from waste and washing of application equipment.

Environmental fate

Dissolution, speciation and partitioning

The basic pKa of the assessed chemical indicates that one to two nitrogen atoms in the assessed chemical are expected to be protonated under environmental pH conditions. The assessed chemical is very water soluble and is not expected to be volatile from waters or moist soils.

The adsorption/desorption result (log Koc = 3.86) provided for LTD/1898 (NICNAS, 2016) indicates that the assessed chemical will readily adsorb to, and be immobile in, soils and sediments. As such, a significant proportion of the assessed chemical released to waters may be expected to adsorb to sediments in waterways or sludge during sewage treatment plant (STP) processes.

Degradation

Degradation studies indicate that the assessed chemical is not readily biodegradable and not hydrolysable.

The biodegradation studies under two OECD guidelines were provided for this application. In a test performed to OECD 301D, 0% degradation was observed after 28 days (GDCM, 2015a). A test performed similar to OECD 301B showed 24% degradation at test concentration of 10 mg/L and 0% degradation at a test concentration of 20 mg/L after 28 days (ESL, 1996).

Hydrolysis information provided for LTD/1898 (NICNAS, 2016) indicates that the assessed chemical is hydrolytically stable with a hydrolysis half-life greater than one year at pH 4, 7, or 9.

Bioaccumulation

The assessed chemical is not expected to bioaccumulate due to its high water solubility (> 50 g/L at 20 °C) and low octanol-water partitioning coefficient (log Kow = 0.446).

Predicted environmental concentration (PEC)

A predicted environmental concentration (PEC) for Australian waters was calculated assuming 5% of the introduction volume was released into sewers and waterways without any removal from STPs. This calculated value is conservative as considerable proportions of the assessed chemical released to waters may be expected to be removed via sludge in STPs.

Total Annual Import Volume	10 000	kg/year
Proportion expected to be released to sewer	5%	
Annual quantity of chemical released to sewer	500	kg/year
Days per year where release occurs	365	days/year
Daily chemical release	1.37	kg/day
Water use	200.0	L/person/day
Population of Australia	24.386	Million
Removal within STP	0%	Mitigation
Daily effluent production	4 877	ML/day
Dilution Factor - River	1.0	
Dilution Factor - Ocean	10.0	
PEC - River	0.28	µg/L
PEC - Ocean	0.028	µg/L

The assessed chemical is not expected to be toxic to terrestrial species (see Environmental effects) and a calculation of a PEC for soils is not required to determine the risk.

Environmental effects

Effects on Aquatic Life

Acute toxicity

The following measured median lethal concentration (LC50), median effective concentration (EC50), and no observable effect concentration (NOEC) values for model organisms were provided for this application:

Taxon	Endpoint	Method
Fish	96 h LC50 ≥ 100 mg/L	*Brachydanio rerio* (zebra fish) OECD TG 203 Semi-static Measured concentration (ESL, 1996)
	96 h LC50 ≥ 100 mg/L	*Giobicypris rarus* (rare minnow) OECD TG 203 Semi-static Measured concentration (GDCM, 2015b)
Invertebrate	48 h EC50 ≥ 320 mg/L	*Daphnia magna* (water flea) Immobility OECD TG 202 Semi-static Measured concentration (ESL, 1996)
	48 h EC50 > 97.5 mg/L	*Daphnia magna* (water flea) Immobility OECD TG 202 Semi-static Measured concentration (ESL, 1996)
Algae	96 h EC50 ≥ 180 mg/L 96 h NOEC = 10 mg/L	*Selenastrum capricornutum* (green algae) growth rate OECD TG 201 Static Measured concentration (ESL, 1996)
Bacteria	16 h EC50 ≥ 300 mg/L; NOEC = 300.9 mg/L	*Pseudomonas putida* ECO SOP 150 02 Growth rate (ESL, 1996)

Based on the above acute toxicity results, the assessed chemical is not expected to be harmful to fish, daphnia and algae.

Effects on terrestrial Life

The following key measured median lethal concentration (LC50) and median effective concentration (EC50) values were provided for this application:

Taxon	Endpoint	Method
Earthworm	14 d LC50 ≥ 100 mg/kg	*Eisenia foetida* OECD TG 207 (ESL, 1996)
Plant	7 d EC50 ≥ 3200 mg/kg	Cress (species not specified) ISO CD 11269-2 growth rate (ESL, 1996)

Predicted no-effect concentration (PNEC)

A predicted no-effect concentration (PNEC) of 0.975 mg/L was calculated for the assessed chemical in the aquatic environment. This value was conservatively derived using the lower bound value for aquatic invertebrates (97.5 mg/L). An assessment factor of 100 was applied to this endpoint as no chronic toxicity data was available.

Categorisation of environmental hazard

The categorisation of the environmental hazards of the assessed chemical according to domestic environmental hazard thresholds is presented below:

Persistence

Based on supplied biodegradation and hydrolysis information, the assessed chemical is categorised as Persistent (P).

Bioaccumulation

Not Bioaccumulative (Not B). Based on low measured log K_{ow} value, and high water solubility, the assessed chemical is categorised as Not Bioaccumulative.

Toxicity

Not Toxic (Not T). Based on available aquatic ecotoxicity endpoints above 1 mg/L, the assessed chemical is categorised as Not Toxic.

Environmental risk characterisation

The assessed chemical is not PBT and is hence unlikely to have unpredictable long-term effects (EPHC 2009). An estimate of risk may therefore be determined using the risk quotient method.

Based on the PEC and PNEC values determined above, Risk Quotients (RQ = PEC ÷ PNEC) have been calculated for release of the assessed chemical to water:

Compartment	PEC	PNEC	RQ
River	0.28 µg/L	975 µg/L	< 0.001
Ocean	0.028 µg/L	975 µg/L	< 0.001

For rivers and oceans, a RQ less than 1 indicates that the assessed chemical is unlikely to cause environmental risk based on estimated emissions, as environmental concentrations are below levels that are likely to cause harmful effects.

For soils, a RQ has not been calculated as the assessed chemical is not expected to be toxic to terrestrial organisms. Therefore, the assessed chemical is unlikely to cause harmful effects in the terrestrial environment.

References

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ESL (1996) Dragon Ligand Chloride: Safety Evaluation Volume 6 of 6 Ecotoxicity (Study No. D96/028, August, 1996). Bedford, England, Environmental Safety Laboratory (Unpublished report submitted by the applicant).

GDCM (2015a) Ready Biodegradability: Closed Bottle Test of Dragon Ligand (Study No. 2015ESG0147, December, 2015). Guangzhou, China, Guangdong Detection Center of Microbiology (Unpublished report submitted by the applicant).

GDCM (2015b) Acute Toxicity Test of Dragon Ligand with Rare Minnow (*Gobiocypris rarus)* (Study No. 2015ESG0148, November, 2015). Guangzhou, China, Guangdong Detection Center of Microbiology (Unpublished report submitted by the applicant).

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