

Nonylphenol ethoxylates and their sulfate and phosphate esters: Environment tier II assessment

25 November 2016

CAS Registry Number: 9016-45-9, 63496-57-1, 68412-54-4, 26027-38-3, 127087-87-0, 27986-36-3, 7311-27-5, 27177-01-1, 27177-05-5, 26571-11-9, 27177-08-8, 51938-25-1, 37205-87-1, 11096-42-7, 9014-90-8, 31691-97-1, 68649-55-8, 63351-73-5, 68511-21-7, 37340-60-6, 68954-84-7, 52503-15-8, 51609-41-7, 51811-79-1, 68412-53-3.



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Preface

This assessment was carried out by staff of the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) using the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework.

The IMAP framework addresses the human health and environmental impacts of previously unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory).

The framework was developed with significant input from stakeholders and provides a more rapid, flexible and transparent approach for the assessment of chemicals listed on the Inventory.

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS

already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

The IMAP framework is a science and risk-based model designed to align the assessment effort with the human health and environmental impacts of chemicals. It has three tiers of assessment, with the assessment effort increasing with each tier. The Tier I assessment is a high throughput approach using tabulated electronic data. The Tier II assessment is an evaluation of risk on a substance-by-substance or chemical category-by-category basis. Tier III assessments are conducted to address specific concerns that could not be resolved during the Tier II assessment.

These assessments are carried out by staff employed by the Australian Government Department of Health and the Australian Government Department of the Environment and Energy. The human health and environment risk assessments are conducted and published separately, using information available at the time, and may be undertaken at different tiers.

This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

For more detail on this program please visit: www.nicnas.gov.au.

Disclaimer

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Acronyms & Abbreviations

Grouping Rationale

This Tier II assessment considers the environmental risks associated with industrial uses of twenty-five substances which are all derivatives of nonylphenol. They are all mixtures of discrete organic chemicals and/or low to moderate molecular weight polymers with ethoxy ether chains. The majority of the substances in this group have component chemicals which are surface active and some substances are industrially important synthetic surfactants. For the purposes of this assessment, they have been sub-grouped into non-ionic ethoxy ether derivatives of nonylphenol (nonylphenol ethoxylates) or the sulfate and phosphate esters of nonylphenol ethoxylates.

The substances in this group have applications in high-volume consumer and commercial cleaning products which will lead to release of the component chemicals into sewers. These chemicals undergo partial degradation in sewage treatment plants into a range of more stable organic chemicals including nonylphenols, which are environmentally hazardous. Hence, industrial uses of the substances in this group can result in emission of both nonylphenol ethoxylates and nonylphenols into the environment in the treated effluents and biosolids produced by sewage treatment plants.

The Tier I assessment of nonylphenol ethoxylate (CAS RN 9016-45-9) and nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8) indicated the potential for unreasonable risks to the environment from their emission to surface waters in treated effluents from sewage treatment plants. This Tier II assessment includes further refinement of the risk characterisation for these

Stage One chemicals and other closely related derivatives of nonylphenol listed on the Inventory. It will also consider the environmental effects of cumulative emissions of their common nonylphenol degradants.

The IMAP Environment Tier II assessment for Nonylphenols (NICNAS, 2016a) has been used as a reference assessment.

Chemical Identity

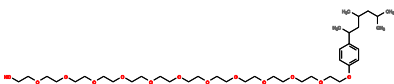
The industrial manufacture of nonylphenol results in a mixture of structural isomers that are substituted with a nonyl (C₉) chain primarily at the *para*- (4-) position of the phenol ring system. Depending on the feedstocks employed, this chain can be either a highly branched nonyl unit or an isononyl unit (NICNAS, 2016a). Hence, all substances in this group will include a mixture of mostly *para*-substituted nonylphenol ethoxylate (or ethoxy ether sulfate or phosphate ester) structural isomers.

Nonylphenol ethoxylates are produced by polymerisation of ethylene oxide (oxirane, CAS RN 75-21-8) with nonylphenols, which results in a mixture of substances with linear ethoxy ether chains of various lengths depending on reaction conditions (Staples, et al., 2008). Commercially available nonylphenol ethoxylates are mixtures of structural isomers and homologues where the ethoxylate chain contains from 1 to 100 ethoxy ether sub-units (Staples, et al., 2008). The chain length of nonylphenol ethoxylate homologues has a normal distribution centred around the average number of ethoxy ether units in the chain (Ahel, et al., 1994a; Staples, et al., 2008). The average non-ionic nonylphenol ethoxylate has a chain comprised of 12 or 13 ethoxy ether sub-units (de Oude, 1992). The ethoxylate chain in anionic derivatives of nonylphenol ethoxylates (including sulfate and phosphate esters) typically contains between 1 and 4 ethoxy ether sub-units (de Oude, 1992).

The structural formula, SMILES string, molecular formula and molecular weight given for each substance are representative of the component chemicals in the mixture. For some substances in this group, only the CAS RN, chemical name and synonyms are presented, as representative chemical structure information is provided for analogous substances in the group.

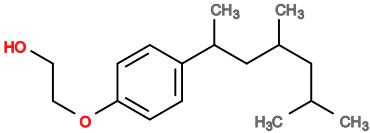
Nonylphenol Ethoxylates

All of the substances in this sub-group are mixtures of nonylphenol ethoxylates with ethoxy ether chains of unspecified lengths unless otherwise indicated.

CAS RN	9016-45-9
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-
Synonyms	nonylphenol ethoxylate
Representative Structural Formula	
Representative Molecular Formula	C ₃₉ H ₇₂ O ₁₃
Representative Molecular Weight (g/mol)	748.98

Representative SMILES	<chem>CC(C)CC(C)CC(C)c1ccc(OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1</chem>
CAS RN	63496-57-1
Chemical Name	Nonyl phenol ethoxylate blend
Synonyms	teric 200
CAS RN	68412-54-4
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, branched
Synonyms	branched nonylphenol ethoxylate
CAS RN	26027-38-3
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(4-nonylphenyl)-.omega.-hydroxy-
Synonyms	nonoxynol <i>p</i> -nonylphenol ethoxylate
CAS RN	127087-87-0
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(4-nonylphenyl)-.omega.-hydroxy-branched
Synonyms	branched <i>p</i> -nonylphenol ethoxylate

This substance is a mixture of nonylphenol ethoxylate isomers with a single ethoxy ether unit. Nonylphenol monoethoxylates are common degradants of longer chain nonylphenol ethoxylates.

CAS RN	27986-36-3
Chemical Name	Ethanol, 2-(nonylphenoxy)-
Synonyms	nonylphenol monoethoxylate
Representative Structural Formula	
Molecular Formula	C ₁₇ H ₂₈ O ₂
Molecular Weight (g/mol)	264.40
Representative SMILES	CC(C)CC(C)CC(C)c1ccc(OCCO)cc1

The substances represented by CAS RNs 7311-27-5, 27177-01-1, 27177-05-5, 26571-11-9 and 27177-08-8 are mixtures of nonylphenol ethoxylates with four, six, eight, nine and ten ethoxy ether units, respectively.

CAS RN	7311-27-5
Chemical Name	Ethanol, 2-[2-[2-[2-(4-nonylphenoxy)ethoxy]ethoxy]ethoxy]-
Synonyms	<i>p</i> -nonylphenol tetraethoxylate

CAS RN	27177-01-1
Chemical Name	3,6,9,12,15-Pentaoxaheptadecan-1-ol, 17-(nonylphenoxy)-
Synonyms	nonylphenol hexaethoxylate

CAS RN	
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27177-05-5

Chemical Name 3,6,9,12,15,18,21-Heptaoxatricosan-1-ol, 23-(nonylphenoxy)-

Synonyms nonylphenol octaethoxylate

CAS RN 26571-11-9

Chemical Name 3,6,9,12,15,18,21,24-Octaoxahexacosan-1-ol, 26-(nonylphenoxy)-

Synonyms nonylphenol nonaethoxylate

CAS RN 27177-08-8

Chemical Name 3,6,9,12,15,18,21,24,27-Nonaoxanonacosan-1-ol, 29-(nonylphenoxy)-

Synonyms nonylphenol decaethoxylate

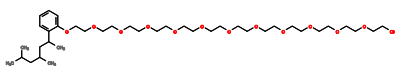
This substance is a mixture of nonylphenol ethoxylates with ethoxy ether chains substituted at the *ortho* position.

CAS RN 51938-25-1

Chemical Name Poly(oxy-1,2-ethanediyl), .alpha.-(2-nonylphenyl)-.omega.-hydroxy-

Synonyms *o*-nonylphenol ethoxylate

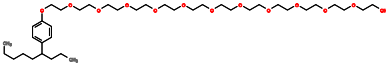
Representative Structural Formula



Representative Molecular Formula $C_{39}H_{72}O_{13}$

Representative Molecular Weight (g/mol)	748.98
Representative SMILES	<chem>CC(C)CC(C)CC(C)c1ccc(OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1</chem>

This substance is a mixture of isononylphenol ethoxylates.

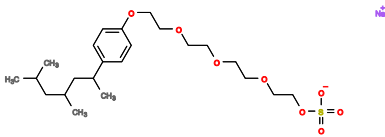
CAS RN	37205-87-1
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(isononylphenyl)-.omega.-hydroxy-
Synonyms	isononylphenol ethoxylate
Representative Structural Formula	
Representative Molecular Formula	C ₃₉ H ₇₂ O ₁₃
Representative Molecular Weight (g/mol)	748.98
Representative SMILES	<chem>CCCCC(CCC)c1ccc(OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1</chem>

This substance is a mixture of nonylphenol ethoxylate adducts of iodine.

CAS RN	11096-42-7
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, compound with iodine
Synonyms	nonylphenol ethoxylate-iodine complex

Nonylphenol Ethoxy Ether Sulfates

All substances in this sub-group are mixtures of inorganic salts of nonylphenol ethoxy ether sulfate esters. The ethoxy ether chains in these substances are of unspecified length, except for the substance identified by CAS RN 63351-73-5. All members of this sub-group may also contain nonylphenol sulfate by-products that are formed from residual nonylphenols present as impurities in the technical nonylphenol ethoxylate starting materials (de Oude, 1992).

CAS RN	9014-90-8
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-(nonylphenoxy)-, sodium salt
Synonyms	nonylphenol ethoxy ether sulfate sodium salt
Representative Structural Formula	
Representative Molecular Formula	C ₂₃ H ₃₉ NaO ₈ S
Representative Molecular Weight (g/mol)	498.61
Representative SMILES	<chem>CC(C)CC(C)CC(C)c1ccc(OCCOCCOCCOCCOS(=O)(=O)[O-])cc1.[Na+]</chem>
CAS RN	31691-97-1
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-(4-nonylphenoxy)-, ammonium salt
Synonyms	<i>p</i> -nonylphenol ethoxy ether sulfate ammonium salt
CAS RN	68649-55-8
Chemical Name	

Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-(nonylphenoxy)-, branched, ammonium salt

Synonyms branched nonylphenol ethoxy ether sulfate ammonium salt

This substance is a mixture of ammonium salts of nonylphenol ethoxy ether sulfates with chains comprised of four ethoxy ether units.

CAS RN 63351-73-5

Chemical Name Ethanol, 2-[2-[2-[2-(nonylphenoxy)ethoxy]ethoxy]ethoxy]-, hydrogen sulfate, ammonium salt

Synonyms nonylphenol triethoxy ether sulfate ammonium salt

Nonylphenol Ethoxy Ether Phosphates

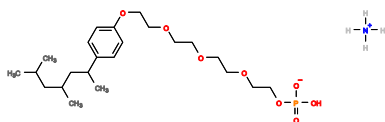
The substances in this group are mixtures of nonylphenol ethoxy ether phosphates or inorganic salts of these organic acids. The ethoxy ether chains in these substances are of unspecified length.

CAS RN 68511-21-7

Chemical Name Poly(oxy-1,2-ethanediyl), alpha -(nonylphenyl)-omega -hydroxy-, phosphate, ammonium salt

Synonyms nonylphenol ethoxy ether phosphate ammonium salt

Representative Structural Formula



Representative Molecular Formula $C_{23}H_{44}NO_8P$

Representative Molecular Weight (g/mol) 493.57

Representative SMILES	<chem>CC(C)CC(C)CC(C)c1ccc(OCCOCCOCCOCCOP(=O)(O)[O-])cc1.[NH4+]</chem>
CAS RN	37340-60-6
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, phosphate, sodium salt
Synonyms	nonylphenol ethoxy ether phosphate sodium salt
CAS RN	68954-84-7
Chemical Name	Poly(oxy-1,2-ethanediyl), a-(nonylphenyl)-w-hydroxy-, branched, phosphates, sodium salts
Synonyms	branched nonylphenol ethoxy ether phosphate sodium salt
CAS RN	52503-15-8
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, phosphate, potassium salt
Synonyms	nonylphenol ethoxy ether phosphate potassium salt
CAS RN	51609-41-7
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(4-nonylphenyl)-.omega.-hydroxy-, phosphate
Synonyms	<i>p</i> -nonylphenol ethoxy ether phosphate

CAS RN	51811-79-1
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, phosphate
Synonyms	nonylphenol ethoxy ether phosphate

CAS RN	68412-53-3
Chemical Name	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-, branched, phosphates
Synonyms	branched nonylphenol ethoxy ether phosphate

Physical and Chemical Properties

Limited measured physical and chemical property data are available for the substances in this group. Experimental data provided for non-ionic nonylphenol ethoxylates below were retrieved from the scientific literature (Mukerjee and Mysels, 1971; Staples, et al., 2008) and the databases included in the OECD QSAR Toolbox and the European Union Registered Substances Database (LMC, 2013; REACH, 2016):

Physical Form	Liquid (less than 10 ethoxy ether units) Solid (greater than 12 ethoxy ether units)
Melting Point	-9°C (1.5 ethoxy ether units) 4°C (9 ethoxy ether units) 42°C (30 ethoxy ether units)
Boiling Point	295–320°C (nonylphenol ethoxylate)
Vapour Pressure	<0.0001 Pa (1.5–30 ethoxy ether units)
Water Solubility	49.6 mg/L (10 ethoxy ether units) 96.9 mg/L (15 ethoxy ether units) 154 mg/L (20 ethoxy ether units)

Ionisable in the Environment?	No
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Most of the substances in this group are composed of mixtures of low to moderate molecular weight organic oligomers or salts and they are therefore expected to have low volatility. The reported water solubility values above are the measured critical micelle concentrations (CMCs) for non-ionic nonylphenol ethoxylates with a reduced distribution of ethoxylate chain lengths centred around 10, 15 and 20 ethoxy ether sub-units, respectively (Mukerjee and Mysels, 1971). The CMCs increase with increasing ethoxylate chain length due to the relatively greater hydrophilicity of longer ethoxylate chains (Environment Canada, 2002).

The octanol-water partition coefficients (K_{OW}) of the chemicals in this group are not considered to be a reliable indicator of the partitioning behaviour of surface-active substances in the environment (McWilliams and Payne, 2001; Shorts, et al., 2010), and are therefore not reported.

The sulfate and phosphate esters of nonylphenol ethoxylates are expected to be strong organic acids based on the acidity of analogue chemicals (Guthrie, 1978). The salts of the nonylphenol ethoxy ether sulfate and phosphate esters in this group are therefore expected to dissociate into their respective sulfate or phosphate ester organic anions and counter cations in water. These organic anions are surface active based on their use as detergents and emulsifiers in a range of product categories (de Oude, 1992).

Import, Manufacture and Use

Australia

Nonylphenol ethoxylate (CAS RN 9016-45-9) is listed on the 2006 High Volume Industrial Chemicals List (HVICL) with a total reported volume of 1000–9999 tonnes. The chemical is used in household products such as cleaning and washing agents (NICNAS, 2016b). It also has a reported commercial use in protective coatings, and site-limited uses as a surface-active agent in the manufacture of other chemicals (NICNAS, 2016b).

p-Nonylphenol ethoxylate (CAS RN 26027-38-3) is reported to be used at less than 1 tonne per year. This chemical has reported commercial uses, including in foam suppressants, de-airing agents, fluorescent whitening agents and paper dyes used by textile dye houses and manufacturers (NICNAS, 2016b).

Nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8) has reported uses in industrial adhesives and tapes.

Nonylphenol ethoxylates and their phosphate ester derivatives are used in Australia as active constituents or excipients in agricultural and veterinary chemical products (APVMA, 2016). However, use of these chemicals in pesticides or veterinary medicines is beyond the scope of this assessment, as such uses are not considered an industrial use under the *Industrial Chemicals (Notification and Assessment) Act 1989*.

No specific Australian use, import, or manufacturing information has been identified for the other chemicals in this group.

International

Chemicals in this group have a wide range of industrial applications, including uses as detergents, emulsifiers, wetting agents and dispersants (Environment Canada, 2002). Household applications include use in cleaning products, paints and cosmetics (Environment Canada, 2002). The sulfate and phosphate esters of nonylphenol ethoxylates in this group are used as anionic detergents, lubricants and antistatic agents (Environment Canada, 2002).

There is also some indication that the chemicals in this group are used in pesticide and pharmaceutical preparations (Environment Canada, 2002). However, such uses are beyond the scope of this assessment.

Environmental Regulatory Status

Australia

The use of the chemicals in this group is not subject to any specific national environmental regulations.

United Nations

The chemicals in this group are not currently identified as Persistent Organic Pollutants (UNEP, 2001), ozone depleting substances (UNEP, 1987), or hazardous substances for the purpose of international trade (UNEP & FAO, 1998).

OECD

Nonylphenol ethoxylate (CAS RN 9016-45-9), branched nonylphenol ethoxylate (CAS RN 68412-54-4) and branched *p*-nonylphenol ethoxylate (CAS RN 127087-87-0) are listed as OECD High Production Volume (HPV) chemicals, indicating that more than 1000 tonnes of the chemicals are produced per year in at least one member country of the OECD (OECD, 2004; 2009).

Nonylphenol ethoxylate (CAS RN 9016-45-9) has been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP), but the assessment has not been completed (OECD, 2013). The remaining chemicals in this group have not been sponsored for assessment under CoCAP (OECD, 2013).

Canada

Nonylphenol ethoxylates are listed under Schedule 1 (the Toxic Substances List) of the *Canadian Environmental Protection Act 1999* (CEPA 1999) (Government of Canada, 2013). Use of nonylphenol ethoxylates has been reduced in Canada since 2004, with most users required to prepare and implement pollution prevention plans. The majority have met risk management objectives by eliminating the use of these chemicals (Environment Canada, 2014).

Most of the chemicals in this group (21 substances) are listed on the Canadian Domestic Substances List (DSL) (Environment Canada, 2013). *p*-Nonylphenol tetraethoxylate (CAS RN 7311-27-5) was found to be Inherently Toxic to the Environment (iT_E). All other listed chemicals were categorised as not Persistent (not P), not Bioaccumulative (not B) and not Inherently Toxic to the Environment (not iT_E).

European Union

A number of chemicals in this group (five substances) are subject to export notification procedures and prior informed consent notification for imports under Regulation No 649/2012 of the European Parliament and of the Council. Importers and exporters of the chemical must notify relevant authorities before transportation of the substance (European Commission, 2012).

Nonylphenol ethoxylates are prohibited for use in the European Union (EU) at concentrations equal to or greater than 0.1% in most cleaning products, or in textile and leather processing, metal working, manufacturing of pulp and paper, cosmetic products and other personal care products under Annex XVII (List of Restrictions) to the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2014). Branched nonylphenol ethoxylate (CAS RN 68412-54-4) is listed on the Community Rolling Action Plan for evaluation under the REACH legislation based on potential for high environmental exposure (ECHA, 2016).

Most of the chemicals in this group (17 substances) have been pre-registered for use in the EU under the REACH legislation (ECHA, 2015a). Nonylphenol ethoxylate (CAS RN 9016-45-9) and branched nonylphenol ethoxylate (CAS RN 68412-54-4) have undergone the full registration process (ECHA, 2015b).

A number of chemicals in this group (four substances: CAS RNs 9014-90-8, 9016-45-9, 26027-38-3 and 27986-36-3) are listed on the European Commission priority list of substances for evaluation of endocrine disruption activity (European Commission,

United States of America

Most of the chemicals in this group (23 substances) are listed on the inventory of chemicals manufactured or processed in the United States of America (USA), as published under the *Toxic Substances Control Act 1976 (TSCA)* (US EPA, 2014a). The United States Environmental Protection Agency (US EPA) published an action plan on nonylphenols and nonylphenol ethoxylates in 2010 (US EPA, 2010a). Significant New Use Rules (SNURs) were subsequently proposed for nine of these chemicals. Under the rules, approval is required before any of these chemicals may be used for new applications (US EPA, 2014b).

Nonylphenol ethoxylate (CAS RN 9016-45-9) and nonylphenol ethoxy ether phosphate (CAS RN 51811-79-1) are listed as United States High Production Volume (US HPV) chemicals, indicating that at least 454 tonnes of the chemicals are manufactured/imported into the USA per year (US EPA, 2010b).

Recently, the US EPA proposed the addition of nonylphenol ethoxylates to the list of toxic chemicals subject to reporting under section 313 of the *Emergency Planning and Community Right-to-Know Act (EPCRA)* and section 6607 of the *Pollution Prevention Act (PPA)*. In the proposed category of nonylphenol ethoxylates, 11 substances in this group are included. Under the proposed rule, those who manufacture, process, or use these chemicals in amounts above reporting threshold levels are required to report their environmental releases and other waste management quantities annually. Pollution prevention and recycling data for these chemicals are also required (United States Government, 2016).

Environmental Exposure

Some chemicals in this group are used in large quantities and have widespread domestic and industrial uses. The most significant industrial use for the chemicals in this group is as a detergent. They are also used as emulsifiers, wetting agents and dispersants. Such use patterns typically result in release of chemicals to sewers. Depending on the degradation and partitioning processes of chemicals in sewage treatment plants (STPs), some fraction of the quantity of chemicals in wastewater entering STPs can be emitted to rivers or oceans in treated effluent, or to soil through application of biosolids to agricultural land (Struijs, 1996). Non-industrial use in pesticide preparations results in direct release of the chemical to the environment, but direct release is not expected from industrial uses.

Removal of anionic surfactants through sorption to sludge, sediment and soil is generally lower than for non-ionic surfactants (Ying, 2006). There are no data available which show the fraction of anionic derivatives of nonylphenol ethoxylates that are removed through sorption to sludge in STPs.

The cationic components (ammonium, sodium, potassium ions) of the chemicals in this group and iodide resulting from reduction of iodine are ubiquitous in the environment. The environmental concentrations of these inorganic species are unlikely to change as a result of the use of the substances in this group. Hence, the environmental fate and effects of the cationic components of the chemicals in this group and iodine are not further considered in this assessment.

Environmental Fate

Partitioning

Short chain nonylphenol ethoxylates are expected to partition between water and sediment, while longer chain nonylphenol ethoxylates are expected to remain in water when released from industrial uses.

Long chain nonylphenol ethoxylates are expected to remain in water as they have high water solubility and low volatility (Nguyen, et al., 2004; Staples, et al., 2008). Water soluble degradation products, nonylphenol ethoxyacetates, are also expected to remain in water (Staples, et al., 2008). In contrast, shorter chain nonylphenol ethoxylates and degradation products such as nonylphenols, nonylphenol mono- and di-ethoxylates have lower water solubility and higher lipophilicity. Hence, they can adsorb to solids such as sediments and sewage sludge more strongly than the parent compounds (Nguyen, et al., 2004 ; NICNAS,

2016a; Ying, 2006). Once adsorbed, they may re-enter the water column through re-suspension of sediment or leaching into ground waters (Environment Canada, 2002).

Degradation

The chemicals in this group are expected to undergo degradation in the environment.

The biodegradation behaviour of the chemicals in this group depends on the environmental conditions (Patoczka and Pulliam, 1990). Recent studies on nonylphenol ethoxylate biotransformation pathways show that under aerobic conditions, nonylphenol ethoxylates undergo rapid primary biodegradation by shortening of the ethoxylate chain followed by oxidation of the terminal alcohol to form nonylphenol ethoxyacetates (Gu, et al., 2010). Under anaerobic conditions, shortening of the ethoxylate chain results in nonylphenols and shorter chain nonylphenol ethoxylate degradants (Lu, et al., 2009). The major degradants are nonylphenoxy acetates and nonylphenol mono-ethoxyacetates, nonylphenol mono- and di-ethoxylates, and to a lesser extent, nonylphenols (Coady, et al., 2010).

Information available for nonylphenol ethoxylate (CAS RN 9016-45-9) was used as representative data to characterise the biodegradability of non-ionic nonylphenol ethoxylates in this group. Nonylphenol ethoxylate undergoes substantial primary biodegradation based on 96% degradation observed after 30 days (Ying, et al., 2002). Degradants (nonylphenol mono- and di-ethoxylates, nonylphenoxy acetate and nonylphenol mono-ethoxyacetate) were generated during the biodegradation process, some of which remained at the end of the assay. While these degradants are much more persistent relative to their parent chemicals, they are expected to be ultimately biodegradable in the environment (Hayashi, et al., 2005; Lu, et al., 2009; NICNAS, 2016a).

Anionic sulfate and phosphate ester derivatives of nonylphenol ethoxylates in this group are biodegradable in water. They can undergo desulfonation or dephosphorylation, following this, the degradation pathway is equivalent to non-ionic nonylphenol ethoxylates. In a study conducted in accordance with OECD Test Guideline (TG) 301C, nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8) showed 31% biochemical oxygen demand (BOD) after 28 days (LMC, 2013).

Bioaccumulation

The chemicals in this group have low to moderate bioaccumulation potential in aquatic organisms.

Nonylphenol ethoxylates are surfactants and most surfactants tend to be retained on epithelial surfaces, rather than cross cellular membranes and bioaccumulate (de Oude, 1992; McWilliams and Payne, 2001). Hence, bioaccumulation for most classes of surfactants is generally below the level for concern (McWilliams and Payne, 2001). This is in agreement with experimental data available for the chemicals in this group.

Information available for nonylphenol ethoxylate (CAS RN 9016-45-9) was used as representative data to determine the bioaccumulation potential of non-ionic nonylphenol ethoxylates in this group. The reported bioconcentration factor (BCF) for this chemical in the fish *Cyprinus carpio* after 42 days was less than 0.2 L/kg at a test concentration of 2 mg/L and less than 1.4 L/kg at a test concentration of 0.2 mg/L (NITE, 2014).

Information available for nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8) was used as representative data to determine the bioaccumulation potential of the remaining anionic surfactants in this group. The reported BCF for this chemical in the fish *Cyprinus carpio* after 42 days was in the range 17 to 53 L/kg at a test concentration of 30 µg/L and less than 150 L/kg at a test concentration of 3 µg/L (NITE, 2014).

In one study, the biomagnification factor (BMF) of nonylphenol ethoxylates was greater than one in bird/fish prey relationships, indicating biomagnification (Hu, et al., 2005). Hu et al. found nonylphenol ethoxylate concentrations in herring gulls to be higher than concentrations in mullet, with a BMF of 2.20. However, it is difficult to interpret the results of this study, as herring gulls often scavenge and dietary nonylphenol ethoxylates may derive from multiple sources. In the absence of further information, these data were not considered to provide sufficient weight of evidence for biomagnification of nonylphenol ethoxylates.

A general association of increasing BCF with decreasing ethoxylate chain length has been reported for nonylphenol ethoxylates, which is attributable to greater hydrophobicity of the shorter chain substances (Environment Canada, 2002). The common degradant of the chemicals in this group, nonylphenol, was determined to have moderate bioaccumulation potential in aquatic and sediment-dwelling organisms (NICNAS, 2016a).

Bioaccumulation data are not available for sediment-dwelling organisms for the chemicals in this group.

Transport

The chemicals in this group are not expected to undergo long-range transport based on their low volatility and biodegradability in the environment.

Nonylphenol ethoxylates are readily sorbed to soil and sediment, which is expected to limit their potential to undergo long-range transport in the environment. Although the substances are soluble in water, nonylphenol ethoxylates have a relatively short primary half-life in water.

Predicted Environmental Concentration (PEC)

Based on domestic monitoring information, common degradants of the chemicals in this group are present in the Australian environment.

The amount of parent nonylphenol ethoxylates released to the environment is expected to be limited as they are eliminated through degradation and removal in STPs (de Oude, 1992). While environmental monitoring studies for the parent nonylphenol ethoxylates are limited, many studies report the wide occurrence of nonylphenol ethoxylate degradants in the environment (Ying, et al., 2002). According to an overseas study, the highest concentration of nonylphenolic compounds observed in river water was nonylphenoxy acetates and nonylphenol ethoxyacetates, followed by nonylphenol mono- and di-ethoxylates, and nonylphenol (Ahel, et al., 1994b).

In a recent study conducted in South-East Queensland, final effluent concentrations of 4-nonylphenol, nonylphenol mono- and di-ethoxylate were in the range of 1.0–3.0 µg/L, 0.80–2.2 µg/L and 0.29–3.0 µg/L, respectively (Ying, et al., 2009). Emissions to surface waters from STPs of these chemicals are expected to result primarily from the biodegradation of chemicals in this group that are released into sewers from their industrial use in a wide range of cleaning and washing products.

No Australian soil monitoring data were located for the chemicals in this group. Overseas monitoring data shows that up to 7214 mg/kg dry weight of alkylphenol ethoxylates was detected in sewage sludge (Harrison, et al., 2006), the majority of which is attributable to nonylphenol ethoxylates (Environment Canada, 2002). This may be an overestimation of Australian environmental concentrations as *p*-nonylphenol concentrations in Australian biosolids are 42% lower than global averages (Langdon, et al., 2011).

Environmental Effects

Effects on Aquatic Life

Nonylphenol monoethoxylate, which is a common degradant of the chemicals in this group and the most toxic member of the group, has the potential to cause toxic effects in aquatic organisms.

Toxicity of nonylphenol ethoxylates is due to their physical surfactant effects. They interact with protein structure, affecting enzymatic function and membrane permeability and thereby cause toxicity to the organism (Coady, et al., 2010). Studies suggest that nonylphenols, short chain nonylphenol ethoxylates and nonylphenol ethoxyacetates act through a common mode of toxic action (Coady, et al., 2010; Environment Canada, 2002; TenEyck and Markee, 2007). They can also act as (o)estrogen agonists to disrupt endocrine functions (Environment Canada, 2002; Ying, et al., 2002).

The currently available ecotoxicity data for nonylphenols are summarised in the IMAP Environment Tier II assessment for Nonylphenols (NICNAS, 2016a). The data indicate high acute aquatic toxicity (median lethal/effective concentration values (LC50/EC50) = 0.069–0.41 mg/L) and chronic toxicity (no-observed-effect concentration values (NOEC) = 0.0074–0.0595 mg/L) in standard ecotoxicity tests.

Acute toxicity

Toxicity of nonylphenol ethoxylate surfactants increases with decreasing ethoxylate chain length (US EPA, 2010c; Ying, 2006). There are limited toxicity data available for chemicals in this group. Data available for nonylphenol ethoxylate (CAS RN 9016-45-9) and nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8) are presented as representative of the long-chain non-ionic and anionic chemicals in this group, respectively. Data for nonylphenol monoethoxylate (CAS RN 27986-36-3), which is a common degradant of the chemicals in this group and the most toxic member of the group, are also presented.

The following measured LC50 and EC50 values for model organisms across three trophic levels were retrieved from the scientific literature (Coady, et al., 2010), and the databases included in the OECD QSAR Toolbox (LMC, 2013) for (a) nonylphenol monoethoxylate (CAS RN 27986-36-3), (b) nonylphenol ethoxylate (CAS RN 9016-45-9), and (c) nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8):

Taxon	Endpoint	Method
Fish	(a) 96 h LC50 = 0.218 mg/L	Experimental <i>Pimephales promelas</i> (Fathead minnow)
	(b) 96 h EC50 = 1.3 mg/L	Experimental <i>Lepomis macrochirus</i> (Bluegill)
	(c) 96 h LC50 = 25.0 mg/L	Experimental <i>Oryzias latipes</i> (Japanese medaka) OECD TG 203
Invertebrates	(a) 48 h EC50 = 0.328 mg/L	Experimental <i>Ceriodaphnia dubia</i> (Water flea)
	(c) 48 h EC50 = 21.0 mg/L	Experimental <i>Daphnia magna</i> (Water flea) OECD TG 202
Algae	(b) 5 d EC50 = 37.4 mg/L	Experimental <i>Scenedesmus opoliensis</i> (Green algae) Static

Taxon	Endpoint	Method
	(c) 72 h EC50 = 25.0 mg/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201

While the chemicals in this group also exhibit microbial toxicity, microbial populations are expected to be acclimatised with respect to nonylphenol ethoxylates under environmental conditions (Karsa and Porter, 1995; Ruiz, et al., 2013)

Chronic toxicity

The following NOEC values for model organisms across two trophic levels were retrieved from the scientific literature (Coady, et al., 2010), and the databases included in the OECD QSAR Toolbox (LMC, 2013) for (a) nonylphenol monoethoxylate (CAS RN 27986-36-3), (b) nonylphenol ethoxylate (CAS RN 9016-45-9), and (c) nonylphenol ethoxy ether sulfate sodium salt (CAS RN 9014-90-8):

Taxon	Endpoint	Method
Fish	(a) 21 d NOEC = 0.048 mg/L	Experimental <i>Oncorhynchus mykiss</i> (Rainbow trout)
Invertebrates	(a) 7 d NOEC = 0.285 mg/L	Experimental <i>Ceriodaphnia dubia</i> (Water flea) Read across from chemical with an average ethoxylate chain length of 1.5
	(b) 6 d NOEC = 1.0 mg/L	Experimental <i>Daphnia magna</i> (Water flea) Prolonged study
Algae	(b) 96 h NOEC = 8.0 mg/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae)

Taxon	Endpoint	Method
	(c) 72 h NOEC = 0.14 mg/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201

Nonylphenols and short chain nonylphenol ethoxylates are known to have endocrine activity and cause toxic effects in the reproductive systems of organisms (Ying, et al., 2002). The chemicals bind to the (o)estrogen receptor and mimic the effects of naturally occurring (o)estrogen (Environment Canada, 2002). However, nonylphenol ethoxylates are less (o)estrogenic than nonylphenols (Klecka, et al., 2008).

Effects on Sediment-Dwelling Life

There are limited sediment toxicity data available for chemicals in this group.

The acute ecotoxicity of nonylphenol ethoxylate (CAS RN 9016-45-9) has been studied for *Capitella capitata* (Gallery worm). A 48 hour LC50 of 3.26 mg/L was obtained for this species under static exposure conditions (LMC, 2013).

Predicted No-Effect Concentration (PNEC)

Fish are the most sensitive taxon to toxic effects of the chemicals in this group, based on the available information. The PNEC derived for the most toxic chemical in this group, nonylphenol monoethoxylate, is 0.48 µg/L based on the 21 d NOEC of 0.048 mg/L for *Oncorhynchus mykiss*. The laboratory chronic toxicity value for this fish species was divided by an assessment factor of 100 to account for both interspecies variation and the relative lack of chronic aquatic toxicity data available for chemicals in this group.

Categorisation of Environmental Hazard

The categorisation of the environmental hazards of the substances in this group according to domestic environmental hazard thresholds is presented below (EPHC, 2009; NICNAS, 2013):

Persistence

Not Persistent (Not P). Based on results obtained from biodegradation studies, all chemicals in this group are categorised as Not Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on the available measured bioconcentration data, all chemicals in this group are categorised as Not Bioaccumulative.

Toxicity

Ethanol, 2-(nonylphenoxy)-

Toxic (T). Based on available acute ecotoxicity values below 1 mg/L and a chronic ecotoxicity value below 0.1 mg/L, this chemical is categorised as Toxic.

All remaining chemicals in this group

Not Toxic (Not T). Based on available acute ecotoxicity values above 1 mg/L and chronic ecotoxicity values above 0.1 mg/L, all remaining chemicals in this group are categorised as Not Toxic.

Summary

Ethanol, 2-(nonylphenoxy)- is categorised as:

- Not P
- Not B
- T

All remaining chemicals in this group are categorised as:

- Not P
- Not B
- Not T

Risk Characterisation

Nonylphenol ethoxylate degradants are more toxic than the parent substances and possess (o)estrogenic activity (Ying, et al., 2002). Given that the parent nonylphenol ethoxylates in this group rapidly degrade to more recalcitrant and toxic common degradants, the environmental risk cannot be adequately characterised based on the parent compounds only. The degradants are expected to have a common toxic mode of action, and hence the additive effects of the degradants observed in Australian STP effluents should be considered.

The major degradants observed in the environment are nonylphenoxy acetates and nonylphenol mono-ethoxyacetates, nonylphenol mono- and di-ethoxylates, and to a lesser extent, nonylphenols (Ahel, et al., 1994b). The relative toxicity of nonylphenoxy acetates and nonylphenol ethoxyacetates is considered to be 100–200 fold less than that of nonylphenols (Coady, et al., 2010; Environment Canada, 2002). Therefore, it is assumed that the primary risk posed by the chemicals in this group results from the release of nonylphenols and nonylphenol mono- and di-ethoxylates to the environment.

The risk posed by the release of nonylphenols is discussed in the IMAP Environment Tier II assessment of Nonylphenols (NICNAS, 2016a). The Risk Quotient ($RQ = PEC \div PNEC$) calculated for nonylphenols was 14.32. The following RQs have been calculated for nonylphenol mono- and di-ethoxylates released into rivers based on the PEC (measured environmental concentrations in this case) and PNEC value determined above:

Chemical	PEC (µg/L)	PNEC (µg/L)	RQ
nonylphenol mono-ethoxylate	0.80–2.2	0.48	1.7–4.6

Chemical	PEC (µg/L)	PNEC (µg/L)	RQ
nonylphenol di-ethoxylate	0.29–3.0	0.48	0.6–6.3

The additive effects of nonylphenol, and nonylphenol mono- and di-ethoxylate give rise to an RQ of up to 25.2 based on the cumulative concentrations of these substances in STP effluents measured in Australia. An RQ of greater than one indicates that industrial uses of the chemicals in this group may pose an unreasonable risk to the aquatic environment, as environmental concentrations may exceed levels that cause harmful effects.

Insufficient data are available to characterise the risks posed by the release of the chemicals in this group to the sediment and soil compartments.

Key Findings

Based on available domestic and international use and exposure information, some substances in this group are widely used in a range of products including cleaning and washing agents, additives and in manufacturing other chemicals. Many of these use patterns can lead to release of the component chemicals into sewage treatment plants.

The substances in this group are susceptible to rapid primary biodegradation, which results in more recalcitrant degradants, some of which are highly toxic to aquatic organisms and have the ability to interfere with the normal functioning of endocrine systems. The cumulative concentration of common degradants from substances in this group measured in Australian STP effluents significantly exceeds the level of concern for aquatic life.

Concerns have been expressed internationally about nonylphenols produced as degradants from the substances in this group. To manage the risks from emission of nonylphenols to the environment, the use of substances in this group has been reduced or eliminated internationally.

The chemicals in this group are not PBT substances according to domestic environmental hazard criteria.

Recommendations

It is recommended that the chemicals in this group be included in the Tier III assessment of nonylphenols, to establish the extent to which these chemicals contribute to nonylphenol ecotoxicity in Australia. Additive effects of the short chain degradation products may also be considered in this assessment.

Environmental Hazard Classification

In addition to the categorisation of environmental hazards according to domestic environmental thresholds presented above, the classification of the environmental hazards of (a) ethanol, 2-(nonylphenoxy)-; (b) poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-; and (c) poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-(nonylphenoxy)-, sodium salt according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) is presented below (UNECE, 2009):

Hazard	GHS Classification (Code)	Hazard Statement
Acute Aquatic	(a) Category 1 (H400)	Very toxic to aquatic life

Hazard	GHS Classification (Code)	Hazard Statement
	(b) Category 2 (H401)	Toxic to aquatic life
	(c) Category 3 (H402)	Harmful to aquatic life
Chronic Aquatic	(a) Category 1 (H410)	Very toxic to aquatic life with long lasting effects
	(b) and (c) Category 2 (H411)	Toxic to aquatic life with long lasting effects

The classification of the aquatic hazards posed by ethanol, 2-(nonylphenoxy)-; poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-; and poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-(nonylphenoxy)-, sodium salt was performed based on the toxicity data presented in this assessment.

The classification of long-term aquatic hazards was performed using the GHS method for substances for which adequate chronic toxicity data are not available, noting the lack of rapid degradability of these chemicals (UNECE, 2007).

The remaining chemicals in this group are not classified in this assessment.

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