Mono- and di-alkyl quaternary ammonium surfactants: Environment tier II assessment

21 April 2016

CAS Registry Number: 112-00-5, 1119-94-4, 4574-04-3, 1119-97-7, 112-02-7, 57-09-0, 505-86-2, 124-03-8, 112-03-8, 17301-53-0, 5538-94-3, 7173-51-5, 2390-68-3, 10361-16-7, 3401-74-9, 1812-53-9, 107-64-2, 123312-54-9, 85409-24-1, 68391-03-7, 106233-03-8, 68607-24-9, 8030-78-2, 61788-78-1, 61789-18-2, 61790-41-8, 68391-06-0, 68424-95-3, 68391-05-9, 68002-59-5, 68783-78-8, 61789-80-8, 68334-33-8, 61789-77-3, 61788-92-9.

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

Acronyms & Abbreviations

Grouping Rationale

This Tier II assessment considers the environmental risks associated with industrial uses of thirty-five mono- and di-alkyl quaternary ammonium salts. All chemicals in this group include an organic cation based on a quaternary nitrogen that is covalently bonded to four alkyl groups including either one or two alkyl chain groups. Although some chemicals in this group are mixtures of salts of organic cations with a range of carbon chain lengths, all cations have at least one alkyl chain that has six or more carbon atoms.

The quaternary ammonium salts in this group dissociate into their respective quaternary ammonium cations and counter anions in water. These quaternary ammonium cations are surfactants which have biocidal activity. They have a wide range of potential domestic and industrial applications, many of which could lead to release of these chemicals into sewers. The chemicals in this group therefore have the potential to be emitted to the environment in treated effluents and biosolids produced by sewage treatment plants.

The Tier I assessment of the Stage One chemicals in this group identified concerns regarding their ecotoxicity and the potential for unreasonable risks to the environment from their emission to surface waters in treated effluents from sewage treatment

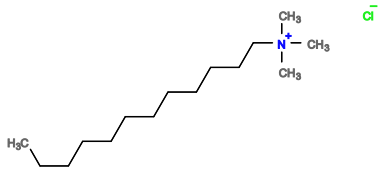
plants. This Tier II assessment includes further refinement of the risk characterisation for these chemicals, together with an assessment of the environmental risks of other closely related quaternary ammonium salts listed on the Inventory.

Chemical Identity

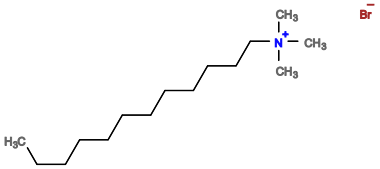
This assessment includes substances composed of a single discrete chemical and substances that are mixtures of discrete chemicals, in the category of unknown or variable composition, complex reaction products or biological materials (UVCBs). The discrete chemicals and mixtures have been sub-grouped for presentation purposes based on similarities in their structures.

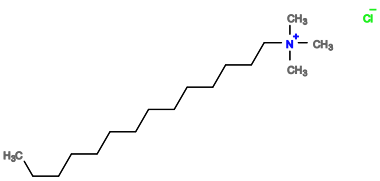
For some UVCBs in this group, only the CAS RN, chemical name and synonyms are presented, as structural information for their component chemicals (or close analogues) are presented under the respective discrete chemical sub-groups. Representative chemical structure information is provided for the main discrete chemical component of UVCBs that are derived from chemicals with biological origins, where composition information for the technical material is available.

Discrete Mono-Alkyl Quaternary Ammonium Surfactants

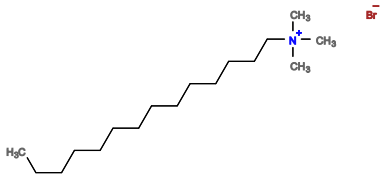
CAS RN	112-00-5
Chemical Name	1-Dodecanaminium, *N*,*N*,*N*-trimethyl-, chloride
Synonyms	dodecyltrimethylammonium chloride lauryltrimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{15}H_{34}ClN$
Molecular Weight (g/mol)	263.90
SMILES	CCCCCCCCCCCC[N+](C)(C)C.[Cl-]

CAS RN	1119-94-4

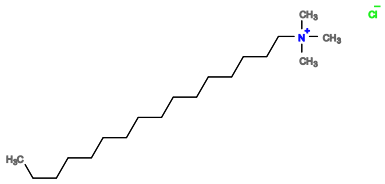
Chemical Name	1-Dodecanaminium, *N*,*N*,*N*-trimethyl-, bromide
Synonyms	dodecyltrimethylammonium bromide lauryltrimethylammonium bromide
Structural Formula	
Molecular Formula	$C_{15}H_{34}BrN$
Molecular Weight (g/mol)	308.35
SMILES	CCCCCCCCCCCC[N+](C)(C)C.[Br-]

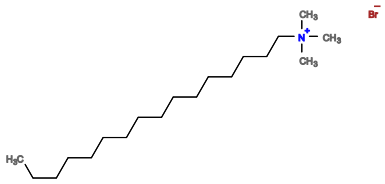
CAS RN	4574-04-3
Chemical Name	1-Tetradecanaminium, *N*,*N*,*N*-trimethyl-, chloride
Synonyms	tetradecyltrimethylammonium chloride myristyltrimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{17}H_{38}ClN$

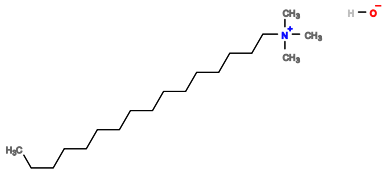
Molecular Weight (g/mol)	291.94
SMILES	CCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]

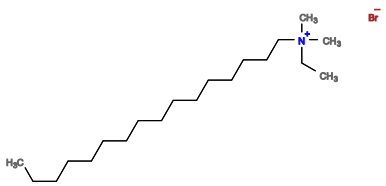
CAS RN	1119-97-7
Chemical Name	1-Tetradecanaminium, *N*,*N*,*N*-trimethyl-, bromide
Synonyms	tetradecyltrimethylammonium bromide myristyltrimethylammonium bromide
Structural Formula	
Molecular Formula	$C_{17}H_{38}BrN$
Molecular Weight (g/mol)	336.39
SMILES	CCCCCCCCCCCCCC[N+](C)(C)C.[Br-]

CAS RN	112-02-7
Chemical Name	1-Hexadecanaminium, *N*,*N*,*N*-trimethyl-, chloride
Synonyms	hexadecyltrimethylammonium chloride cetyltrimethylammonium chloride

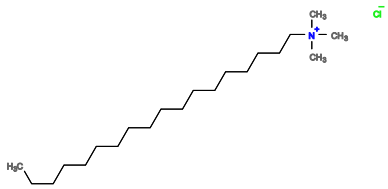
Structural Formula	
Molecular Formula	$C_{19}H_{42}ClN$
Molecular Weight (g/mol)	320.01
SMILES	CCCCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]

CAS RN	57-09-0
Chemical Name	1-Hexadecanaminium, *N*,*N*,*N*-trimethyl-, bromide
Synonyms	hexadecyltrimethylammonium bromide cetyltrimethylammonium bromide
Structural Formula	
Molecular Formula	$C_{19}H_{42}BrN$
Molecular Weight (g/mol)	364.46
SMILES	CCCCCCCCCCCCCCCC[N+](C)(C)C.[Br-]

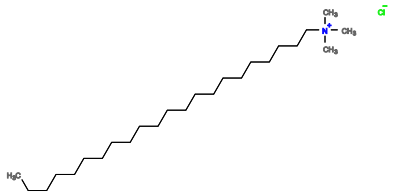
CAS RN	505-86-2
Chemical Name	1-Hexadecanaminium, *N*,*N*,*N*-trimethyl-, hydroxide
Synonyms	hexadecyltrimethylammonium hydroxide cetyltrimethylammonium hydroxide
Structural Formula	
Molecular Formula	$C_{19}H_{43}NO$
Molecular Weight (g/mol)	301.55
SMILES	CCCCCCCCCCCCCCCC[N+](C)(C)C.[OH-]

CAS RN	124-03-8
Chemical Name	1-Hexadecanaminium, *N*-ethyl-*N*,*N*-dimethyl-, bromide
Synonyms	ethylhexadecyldimethylammonium bromide cetyldimethylethylammonium bromide
Structural Formula	
Molecular Formula	$C_{20}H_{44}BrN$

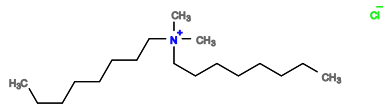
Molecular Weight (g/mol)	378.47
SMILES	CCCCCCCCCCCCCCCC[N+](CC)(C)(C).[Br-]

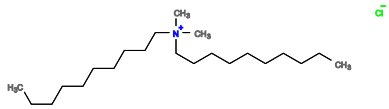
CAS RN	112-03-8
Chemical Name	1-Octadecanaminium, *N*,*N*,*N*-trimethyl-, chloride
Synonyms	octadecyltrimethylammonium chloride stearyltrimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{21}H_{46}ClN$
Molecular Weight (g/mol)	348.06
SMILES	CCCCCCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]

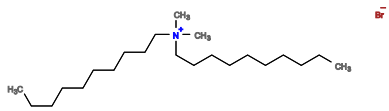
CAS RN	17301-53-0
Chemical Name	1-Docosanaminium, *N*,*N*,*N*-trimethyl-, chloride
Synonyms	docosyltrimethylammonium chloride

	behenyltrimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{25}H_{54}ClN$
Molecular Weight (g/mol)	404.17
SMILES	CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]

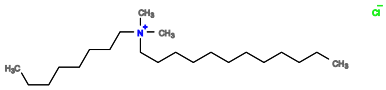
Discrete Di-Alkyl Quaternary Ammonium Surfactants

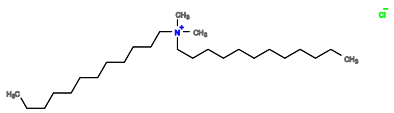
CAS RN	5538-94-3
Chemical Name	1-Octanaminium, *N*,*N*-dimethyl-*N*-octyl-, chloride
Synonyms	dioctyldimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{18}H_{40}ClN$
Molecular Weight (g/mol)	305.97
SMILES	CCCCCCCC[N+](CCCCCCCC)(C)(C).[Cl-]

CAS RN	7173-51-5
Chemical Name	1-Decanaminium, *N*-decyl-*N*,*N*-dimethyl-, chloride
Synonyms	didecyldimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{22}H_{48}ClN$
Molecular Weight (g/mol)	362.09
SMILES	CCCCCCCCCC[N+](CCCCCCCCCC)(C)(C).[Cl-]

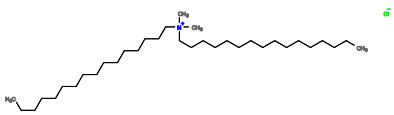
CAS RN	2390-68-3
Chemical Name	1-Decanaminium, *N*-decyl-*N*,*N*-dimethyl-, bromide
Synonyms	didecyldimethylammonium bromide
Structural Formula	
Molecular Formula	$C_{22}H_{48}BrN$
Molecular Weight (g/mol)	406.53

SMILES	CCCCCCCCCC[N+](CCCCCCCCCC)(C)(C).[Br-]

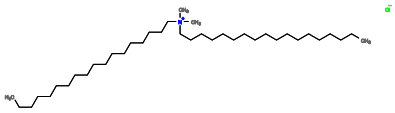
CAS RN	10361-16-7
Chemical Name	1-Dodecanaminium, *N*,*N*-dimethyl-*N*-octyl-, chloride
Synonyms	dodecyloctyldimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{22}H_{48}ClN$
Molecular Weight (g/mol)	362.08
SMILES	CCCCCCCC[N+](CCCCCCCCCCCC)(C)(C).[Cl-]

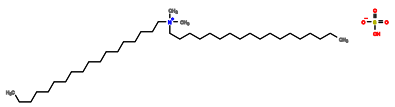
CAS RN	3401-74-9
Chemical Name	1-Dodecanaminium, *N*-dodecyl-*N*,*N*-dimethyl-, chloride
Synonyms	didodecyldimethylammonium chloride dilauryldimethylammonium chloride
Structural Formula	

Molecular Formula	$C_{26}H_{56}ClN$
Molecular Weight (g/mol)	418.18
SMILES	CCCCCCCCCCCC[N+](CCCCCCCCCCCC)(C)(C).[Cl-]

CAS RN	1812-53-9
Chemical Name	1-Hexadecanaminium, *N*-hexadecyl-*N*,*N*-dimethyl-, chloride
Synonyms	dihexadecyldimethylammonium chloride dicetyldimethylammonium chloride
Structural Formula	
Molecular Formula	$C_{34}H_{72}ClN$
Molecular Weight (g/mol)	530.40
SMILES	CCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCCCCCC)(C)(C).[Cl-]

CAS RN	107-64-2
Chemical Name	1-Octadecanaminium, *N*,*N*-dimethyl-*N*-octadecyl-, chloride
Synonyms	dioctadecyldimethylammonium chloride distearyldimethylammonium chloride

Structural Formula	
Molecular Formula	$C_{38}H_{80}ClN$
Molecular Weight (g/mol)	586.50
SMILES	CCCCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCCCCCCCC)(C)(C).[Cl-]

CAS RN	123312-54-9
Chemical Name	1-Octadecanaminium, *N*,*N*-dimethyl-*N*-octadecyl-, sulfate (1:1)
Synonyms	dioctadecyldimethylammonium bisulfate distearyldimethylammonium bisulfate
Structural Formula	
Molecular Formula	$C_{38}H_{81}NO_4S$
Molecular Weight (g/mol)	648.12
SMILES	CCCCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCCCCCCCC)(C)(C).OS(=O)(=O)[O-]

UVCB Mono-Alkyl Quaternary Ammonium Surfactants

The substance represented by CAS RN 85409-24-1 is expected to be a mixture of discrete chemicals with alkyl chains of 12 to 14 carbons.

CAS RN	85409-24-1
Chemical Name	Quaternary ammonium compounds, C12-14-alkyltrimethyl, chlorides
Synonyms	C_{12-14}-alkyltrimethylammonium chlorides

The substance represented by CAS RN 68391-03-7 is expected to be a mixture of discrete chemicals with alkyl chains of 12 to 18 carbons.

CAS RN	68391-03-7
Chemical Name	Quaternary ammonium compounds, C12-18-alkyltrimethyl, chlorides
Synonyms	C_{12-18}-alkyltrimethylammonium chlorides

The substance represented by CAS RN 106233-03-8 is expected to be a mixture of discrete chemicals with alkyl chains of 16 to 24 carbons.

CAS RN	106233-03-8
Chemical Name	Quaternary ammonium compounds, C16-24-alkyltrimethyl, chlorides
Synonyms	C_{16-24}-alkyltrimethylammonium chlorides

The substance represented by CAS RN 68607-24-9 is expected to be a mixture of discrete chemicals with alkyl chains of 20 to 22 carbons.

CAS RN	68607-24-9
Chemical Name	Quaternary ammonium compounds, C20-22-alkyltrimethyl, chlorides

Synonyms	C_{20-22}-alkyltrimethylammonium chlorides

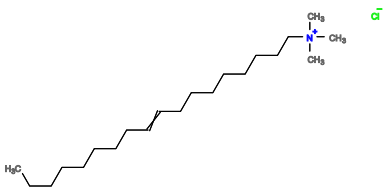
The remaining UVCBs in this sub-group are quaternary ammonium salts that are derived from chemicals that have a biological origin.

Commercially available quaternary ammonium surfactants are often prepared indirectly from natural fats and oils. Natural fats derived from the fatty tissue of sheep or cattle, oil obtained from the kernel of the seed of *Cocos nucifera* (coconut), and seeds of *Glycine soja* (soybean) are used to prepare tallow alkyl-, coconut oil alkyl-, and soybean oil alkyl-ammonium compounds, respectively (Ash and Ash, 2004a; b). These surfactants have carbon chains with even numbers of carbon atoms, as fatty acid biosynthesis occurs mainly through addition of two carbon units in the form of acetyl-CoA (Voet and Voet, 1990).

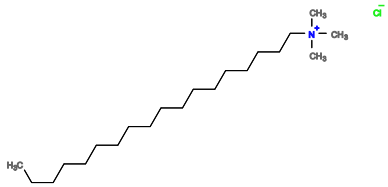
The major process for transforming fats and oils of biological origins into oleochemicals is the hydrolysis of natural triglycerides into glycerine and mixed fatty acids (Corma, et al., 2007). Reaction of these fatty acids and ammonia followed by hydrogenation produces fatty amines (Corma, et al., 2007), which are then alkylated at the nitrogen atom by reaction with chloromethane (CAS RN 74-87-3) (de Oude, 1992). Alternatively, the fatty acids may be reacted with trimethylamine (CAR RN 75-50-3) followed by hydrogenation to form quaternary ammonium compounds (Qadir, et al., 2014).

Representative chemical identity information for the remaining substances in this sub-group is provided below for the discrete chemical that is expected to be most abundant in the technical mixture based on the reported composition of their respective fatty amine precursors (ECHA, 2016a).

The substance represented by CAS RN 8030-78-2 is expected to be a mixture of discrete chemicals with alkyl chains of 12 to 18 carbons derived from tallow.

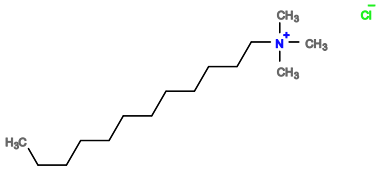
CAS RN	8030-78-2
Chemical Name	Quaternary ammonium compounds, trimethyl tallow alkyl, chlorides
Synonyms	tallow alkyltrimethylammonium chloride
Representative Structural Formula	
Representative Molecular Formula	$C_{21}H_{44}ClN$
Representative Molecular Weight (g/mol)	346.03
Representative SMILES	CCCCCCCCC=CCCCCCCCC[N+](C)(C)C.[Cl-]

The substance represented by CAS RN 61788-78-1 is expected to be a mixture of discrete chemicals with alkyl chains of 12 to 18 carbons derived from hydrogenated tallow.

CAS RN	61788-78-1
Chemical Name	Quaternary ammonium compounds, (hydrogenated tallow alkyl)trimethyl, chlorides
Synonyms	(hydrogenated tallow alkyl)trimethylammonium chloride
Representative Structural Formula	
Representative Molecular Formula	$C_{21}H_{46}ClN$
Representative Molecular Weight (g/mol)	348.06
Representative SMILES	CCCCCCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]

The substance represented by CAS RN 61789-18-2 is expected to be a mixture of discrete chemicals with alkyl chains of six to 18 carbons derived from coconut oil.

CAS RN	61789-18-2
Chemical Name	Quaternary ammonium compounds, coconut alkyltrimethyl, chlorides
Synonyms	(coconut oil alkyl)trimethylammonium chloride

Representative Structural Formula	
Representative Molecular Formula	$C_{15}H_{34}ClN$
Representative Molecular Weight (g/mol)	263.90
Representative SMILES	CCCCCCCCCCCC[N+](C)(C)C.[Cl-]

The substance represented by CAS RN 61790-41-8 is expected to be a mixture of discrete chemicals with saturated and unsaturated alkyl chains of 16 to 18 carbons derived from soybean oil.

CAS RN	61790-41-8
Chemical Name	Quaternary ammonium compounds, trimethylsoya alkyl, chlorides
Synonyms	(soybean oil alkyl)trimethylammonium chloride

UVCB Di-Alkyl Quaternary Ammonium Surfactants

The substance represented by CAS RN 68391-06-0 is expected to be a mixture of discrete chemicals with two alkyl chains of six to 12 carbons.

CAS RN	68391-06-0
Chemical Name	Quaternary ammonium compounds, di-C6-12-alkyldimethyl, chlorides
Synonyms	di-C_{6-12}-dialkyldimethylammonium chlorides

The substance represented by CAS RN 68424-95-3 is expected to be a mixture of discrete chemicals with two alkyl chains of eight to 10 carbons.

CAS RN	68424-95-3
Chemical Name	Quaternary ammonium compounds, di-C8-10-alkyldimethyl, chlorides
Synonyms	di-C_{8-10}-alkyldimethylammonium chlorides

The substance represented by CAS RN 68391-05-9 is expected to be a mixture of discrete chemicals with two alkyl chains of 12 to 18 carbons.

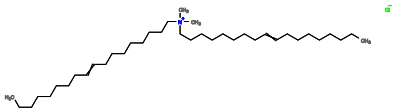
CAS RN	68391-05-9
Chemical Name	Quaternary ammonium compounds, di-C12-18-alkyldimethyl, chlorides
Synonyms	di-C_{12-18}-alkyldimethylammonium chlorides

The substance represented by CAS RN 68002-59-5 is expected to be a mixture of discrete chemicals with two alkyl chains of 14 to 18 carbons.

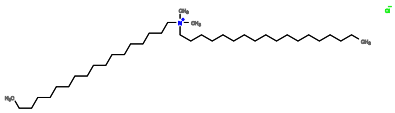
CAS RN	68002-59-5
Chemical Name	Quaternary ammonium compounds, di-C14-18-alkyldimethyl, chlorides
Synonyms	di-C_{14-18}-alkyldimethylammonium chlorides

The substance represented by CAS RN 68783-78-8 is expected to be a mixture of discrete chemicals with two saturated or unsaturated alkyl chains of 12 to 18 carbons derived from tallow.

CAS RN	68783-78-8
Chemical Name	Quaternary ammonium compounds, dimethyl ditallow alkyl, chlorides

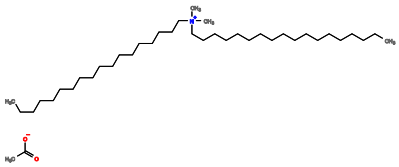
Synonyms	ditallowdimethylammonium chlorides
Representative Structural Formula	
Representative Molecular Formula	$C_{38}H_{76}ClN$
Representative Molecular Weight (g/mol)	582.47
Representative SMILES	CCCCCCCCC=CCCCCCCCC[N+](CCCCCCCCC=CCCCCCCCC)(C)(C).[Cl-]

The substance represented by CAS RN 61789-80-8 is expected to be a mixture of discrete chemicals with two alkyl chains of 12 to 18 carbons derived from hydrogenated tallow.

CAS RN	61789-80-8
Chemical Name	Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, chlorides
Synonyms	bis(hydrogenated tallow alkyl)dimethylammonium chlorides
Representative Structural Formula	
Representative Molecular Formula	$C_{38}H_{80}ClN$
Representative Molecular Weight (g/mol)	586.50

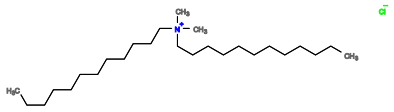
Representative SMILES	CCCCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCCCCCCCC)(C)(C).[Cl-]

The substance represented by CAS RN 68334-33-8 is expected to be a mixture of discrete chemicals with two alkyl chains of 12 to 18 carbons derived from hydrogenated tallow.

CAS RN	68334-33-8
Chemical Name	Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, acetates
Synonyms	bis(hydrogenated tallow alkyl)dimethylammonium acetate
Representative Structural Formula	
Representative Molecular Formula	$C_{40}H_{83}NO_2$
Representative Molecular Weight (g/mol)	610.09
Representative SMILES	CCCCCCCCCCCCCCCCCC[N+](CCCCCCCCCCCCCCCCCC)(C)(C).O=C([O-])C

The substance represented by CAS RN 61789-77-3 is expected to be a mixture of discrete chemicals with two alkyl chains of six to 18 carbons derived from coconut oil.

CAS RN	61789-77-3
Chemical Name	Quaternary ammonium compounds, dicoco alkyldimethyl, chlorides
Synonyms	bis(coconut oil alkyl)dimethylammonium chloride

Representative Structural Formula	
Representative Molecular Formula	$C_{26}H_{56}ClN$
Representative Molecular Weight (g/mol)	418.18
Representative SMILES	CCCCCCCCCCCC[N+](CCCCCCCCCCCC)(C)(C).[Cl-]

The substance represented by CAS RN 61788-92-9 is expected to be a mixture of discrete chemicals with two saturated and unsaturated alkyl chains of 16 to 18 carbons derived from soybean oil.

CAS RN	61788-92-9
Chemical Name	Quaternary ammonium compounds, dimethyldisoya alkyl, chlorides
Synonyms	bis(soybean oil alkyl)dimethylammonium chloride

Physical and Chemical Properties

The measured physical and chemical property data for the chemicals in this group were retrieved from the scientific literature (Kopecky, et al., 2007; Mukerjee and Mysels, 1971; Tezel, 2009), and the databases included in the OECD QSAR Toolbox and the United States National Library of Medicine Hazardous Substances Data Bank (LMC, 2013; US NLM, 2013):

Chemical class	Mono-alkyl quaternary ammonium compounds	Di-alkyl quaternary ammonium compounds
Physical Form	Solid	Solid
Melting Point	240°C (C_{16}) (exp.)	94°C (C_{10}:C_{10}) (exp.)

Water Solubility	5280 mg/L (C_{12}) (exp.) 450 mg/L (C_{16}) (exp.) 100 mg/L (C_{18}) (exp.)	5040 mg/L (C_8:C_8) (exp.) 540 mg/L (C_{10}:C_{10}) (exp.) 40 mg/L (C_{12}:C_{12}) (exp.)
Ionisable in the Environment?	Yes	Yes

The chemicals in this group are all salts of quaternary ammonium surfactants and are therefore expected to have low volatility (de Oude, 1992). The water solubility values reported were determined at the critical micelle concentrations (CMCs), as is appropriate for surface-active substances. CMCs decrease with increasing alkyl chain lengths, and di-alkyl quaternary ammonium compounds have lower CMCs compared to mono-alkyl quaternary ammonium compounds with comparable alkyl chain lengths (Tezel, 2009).

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

Import, Manufacture and Use

Australia

Di-alkyl quaternary ammonium compounds (di-$C_{8\text{-}10}$-alkyldimethylammonium chlorides, didecyldimethylammonium chloride and dioctyldimethylammonium chloride) are used in Australia as active constituents 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 use is not considered an industrial use under the *Industrial Chemicals (Notification and Assessment) Act 1989*.

Dodecyltrimethylammonium bromide has reported commercial use in automotive coatings.

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

International

Chemicals in this group are a source of cationic surfactants that have a wide range of industrial applications reported internationally. They are used in cleaning and washing agents as well as cosmetics, such as hair conditioners, hand soaps and deodorants (SYKE, 2014; US EPA, 2015). Due to their biocidal activity, they are used in agricultural and non-agricultural pesticides, disinfectants and preservatives (Nordic Council of Ministers, 2015; US EPA, 2015). There is also some indication of use as algaecides, indicating potential water treatment uses (US EPA, 2015; US NLM, 2011). However, algaecide use is beyond the scope of this assessment as such use is not considered an industrial use under the *Industrial Chemicals (Notification and Assessment) Act 1989*.

During the 1990s, the production of ditallowdimethylammonium chlorides (CAS RN 68783-78-8) and the structurally related di-alkyl quaternary ammonium compounds with C_{18} alkyl chains was voluntarily replaced in several countries by readily biodegradable quaternary ammonium salts containing ester groups (Madsen, et al., 2001; Ying, 2006; Zhang, et al., 2015).

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

A number of chemicals in this group (11 substances) 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).

Only one chemical in this group (dioctadecyldimethylammonium chloride) has been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP) (OECD, 2013). In the EU risk assessment report, no need for further work was identified (IHCP, 2009).

Canada

The chemicals in this group are not listed under Schedule 1 (the Toxic Substances List) of the *Canadian Environmental Protection Act 1999* (CEPA 1999) (Government of Canada, 2013b).

Most of the chemicals in this group (22 substances) are listed on the Canadian Domestic Substances List (DSL) (Environment Canada, 2013). Most of the listed chemicals (12 substances) were found to be Inherently Toxic to the Environment (iT_E). Only one of the listed chemical (bis(coconut oil alkyl)dimethylammonium chloride) was found to be Inherently Toxic to the Environment (iT_E) and Bioaccumulative (B). Another listed chemical, hexadecyltrimethylammonium bromide, was found to be Inherently Toxic to the Environment (iT_E) and Persistent (P). Four chemicals, hexadecyltrimethylammonium bromide, di-C_{12-18}-alkyldimethylammonium chlorides, bis(hydrogenated tallow alkyl)dimethylammonium chlorides, and bis(coconut oil alkyl)dimethylammonium chloride) are prioritised for further assessment under the Chemicals Management Plan (CMP) (Government of Canada, 2013a).

European Union

Most of the chemicals in this group (32 substances) have been pre-registered for use in the European Union under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation (ECHA, 2015b). Some of the pre-registered chemicals (11 substances) have undergone the full registration process (ECHA, 2015c).

United States of America

Most of the chemicals in this group (29 substances) are listed on the inventory of chemicals manufactured or processed in the USA, as published under the *Toxic Substances Control Act 1976* (TSCA) (US EPA, 2014).

A number of chemicals (11 substances) in this group 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, 2010a).

Environmental Exposure

Chemicals in this group have widespread domestic and industrial uses, many of which result in eventual release of the chemicals into sewage treatment plants (STPs). Depending on degradation and partitioning processes of chemicals in 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; Zhang, et al., 2015).

Based on the partitioning properties of quaternary ammonium compounds, approximately 90% of the total volume of these chemicals entering a typical STP may be removed by adsorption to sludge (Games, et al., 1982), which may be applied to land as biosolids. Hence, emissions of chemicals in this group to both environmental surface waters and soils are considered as part of this assessment.

The anionic components (chloride, bromide, hydroxide, sulfate and acetate ions) of the chemicals in this group are naturally occurring in the environment, and the background concentrations of these species are unlikely to be perturbed by their use as counterions in the substances of this group. Hence, the environmental fate and effects of the anionic components of the chemicals in this group are not considered in this assessment.

Environmental Fate

Dissolution, Speciation and Partitioning

The quaternary ammonium cations from substances in this group partition between water and sediment, or remain in soil when released from industrial uses.

The chemicals in this group are quaternary ammonium salts. If discharged into natural waters, the chemicals are expected to dissociate and release their quaternary ammonium cations. The quaternary ammonium cations can adsorb to clays and natural organic materials, such as humic substances (de Oude, 1992). They are expected to remain in soil as they are strongly adsorbed and immobile (Zhang, et al., 2015).

Degradation

The quaternary ammonium cations from substances in this group are biodegradable.

There are numerous biodegradation studies available for chemicals in this group with a range of biodegradabilities (0–100%) reported based on dissolved organic carbon (DOC) removal, biochemical oxygen demand (BOD), chemical oxygen demand (COD) and CO_2 evolution. The degradation pathway for alkyl quaternary ammonium cations is considered to be via *N*-dealkylation, followed by *N*-demethylation (Ying, 2006). Those chemicals with longer alkyl chains are relatively more persistent (Madsen, et al., 2001), and di-alkyl quaternary ammonium chemicals are generally more recalcitrant than the mono-alkyl derivatives (de Oude, 1992; Ying, 2006).

Although long-chain dialkyl quaternary ammonium compounds have been replaced by more degradable analogues in the past, more recent studies suggest higher degradation potential for these chemicals under environmental conditions (Madsen, et al., 2001). In the environment, microbial populations are expected to be acclimatised to commonly used quaternary ammonium cations, and bacterial toxicity is greatly reduced through quaternary ammonium cations binding to anionic surfactants in sewage (Boethling, 1984; de Oude, 1992).

Mono-alkyl quaternary ammonium compounds in this group are biodegradable in water, including those with the longest alkyl chains. In a study conducted in accordance with OECD Test Guideline (TG) 301B, mono-alkyl quaternary ammonium compound with a C_{16} alkyl chain (CAS RN 112-02-7) showed 93.5% CO_2 evolution after 28 days (ECHA, 2016b), indicating rapid biodegradability. In another ready biodegradation test conducted in accordance with OECD TG 301E, mono-alkyl quaternary ammonium compounds with $C_{20\text{-}22}$ alkyl chains showed O_2 consumption of 50% of theoretical oxygen demand in 28 days (ECHA, 2016a), indicating that mono-alkyl quaternary ammonium compounds with the longest alkyl chains are at least ultimately biodegradable.

Di-alkyl quaternary ammonium cations are also found to be rapidly biodegradable in water, undergoing 79 to 80% degradation after 2 days for those with $C_{12\text{-}18}$ alkyl chains (CAS RNs 61789-80-8 and 61789-77-3) (US EPA, 2016).

Mono-alkyl quaternary ammonium cations are not persistent in soil. Following OECD TG 304A, the biodegradation of mono-alkyl quaternary ammonium compound with a C_{16} alkyl chain (CAS RN 57-09-0) undergoes 60% degradation in 58 days based on $^{14}CO_2$ evolution from ^{14}C-labelled substances added to the soil (ECHA, 2015a).

Bioaccumulation

The quaternary ammonium cations from substances in this group have low to moderate bioaccumulation potential in aquatic organisms.

Quaternary ammonium cations are surfactants and 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.

Most surfactants tend to be retained on epithelial surfaces, rather than cross cellular membranes and bioaccumulate (de Oude, 1992; McWilliams and Payne, 2001). Reported bioconcentration factor (BCF) values are often overestimated as differentiating between parent compounds and metabolites or other breakdown products is difficult for experimental studies with radiolabelled compounds (McWilliams and Payne, 2001).

The reported BCF for a mono-alkyl quaternary ammonium compound with a C_{16} alkyl chain (CAS RN 57-09-0) in the fish *Cyprinus carpio* was in the range of 407 to 741 L/kg at a test concentration of 0.05 mg/L and 444 to 677 L/kg at a test concentration of 0.005 mg/L (NITE, 2014). A general association of increasing alkyl chain length with an increase in BCF has been reported for mono-alkyl quaternary ammonium compounds (Tolls, et al., 1994).

The reported BCF for a di-alkyl quaternary ammonium compound with C_{10} alkyl chains (CAS RN 7173-51-5) in the fish *Cyprinus carpio* is 63 L/kg at a test concentration of 0.005 mg/L and in the range of 47 to 95 L/kg at a test concentration of 0.0005 mg/L (NITE, 2014).

Information available for the mixture of di-alkyl quaternary ammonium compounds with $C_{12\text{-}20}$ alkyl chains was used as representative data to determine the bioaccumulation potential of the remaining di-alkyl quaternary ammonium cations in this group. The reported BCF for di-alkyl quaternary ammonium compounds with $C_{12\text{-}20}$ alkyl chains in the fish *Lepomis macrochirus* is 13 L/kg at a mean test concentration of 0.018 mg/L (IHCP, 2009).

Bioaccumulation also appears low in sediment-dwelling organisms. The 28-day biota sediment accumulation factor (BSAF) for a di-alkyl quaternary ammonium compound with C_{18} alkyl chains (CAS RN 107-64-2) is 0.28 in the worm *Lumbriculus variegatus* (IHCP, 2009). The ingestion of sediment was identified as a key exposure pathway in this study.

Transport

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

Quaternary ammonium cations adsorbed to clays, sediment and soil containing organic carbon (de Oude, 1992; Ivankovic and Hrenovic, 2010) are strongly bound and immobile (Zhang, et al., 2015).

Predicted Environmental Concentration (PEC)

Predicted environmental concentrations for the chemicals in this group were estimated using standard exposure modelling.

No Australian environmental monitoring data were located for the chemicals in this group. According to overseas monitoring data across multiple sewage treatment plants, high removal efficiency of 90% or greater is obtained for quaternary ammonium surfactants (de Oude, 1992; Games, et al., 1982). Once removed, biodegradation occurs on sludge solids (de Oude, 1992). Based on introduction volumes of 100 tonnes per annum (reported or default, in accordance with the IMAP Framework (NICNAS, 2013)), standard Australian exposure modelling parameters (EPHC, 2009), and assuming 90% removal at the sewage treatment plant, the PEC in receiving waters is calculated to be 8.5 µg/L for each chemical in this group.

However, available international monitoring data suggest that these PEC values may overestimate actual environmental exposure concentrations in Australia. A recent review of environmental monitoring studies for quaternary ammonium compounds has reported the concentration of these compounds in sewage, sludge, surface water and sediment across a number of countries including China, Taiwan, Poland, Austria, Spain, England and the USA (Zhang, et al., 2015). The total concentration of mono-alkyl quaternary ammonium compounds with C_{12-18} alkyl chains measured in Taiwanese river water was up to 1.24 µg/L, while the concentration of each di-alkyl quaternary ammonium compound measured in Austrian surface water was up to 0.19 µg/L. On average, the total concentration of quaternary ammonium compounds measured in different urban estuarine sediments in the USA is 29 µg/g (Zhang, et al., 2015).

Environmental Effects

Effects on Aquatic Life

The chemicals in this group have the potential to cause toxic effects in aquatic organisms across multiple trophic levels depending on the bioavailability of the surface-active quaternary ammonium cations.

Algae and invertebrates were found to be most sensitive to toxic effects of quaternary ammonium surfactants. Toxicity of quaternary ammonium compounds to aquatic organisms is not due to bioaccumulation, but due to membrane surfaces being disrupted by the alkyl chains of cationic surfactants, which results in a loss of membrane integrity (McWilliams and Payne, 2001; Zhang, et al., 2015).

In general, laboratory-derived toxicity values are many times lower than field toxicity values (de Oude, 1992), which suggests that quaternary ammonium cations are largely sorbed to particulate matter and become less bioavailable under environmental conditions.

Acute toxicity

Toxicity of mono-alkyl quaternary ammonium surfactants increases with increasing alkyl chain length up to C_{16}, and then decreases (US EPA, 2010b). Due to insufficient toxicity data available for all chemicals in the group, data available for a mono-alkyl quaternary ammonium compound with a C_{16} alkyl chain are presented as representative toxicity data for analogous chemicals in this group.

Information available for di-alkyl quaternary ammonium compounds with C_{10} alkyl chains and those with C_{18} alkyl chains are presented as representative data for the di-alkyl quaternary ammonium compounds in this group. As observed with the mono-alkyl ammonium compounds, di-alkyl quaternary ammonium compounds with the longest alkyl chains have decreased toxicity.

The following measured median lethal concentration (LC50) and median effective concentration (EC50) values for model organisms across three trophic levels were reported in the Screening-Level Hazard Characterisation conducted by the United States Environmental Protection Agency (US EPA, 2008), the European Union Risk Assessment Report (IHCP, 2009), and the databases included in the OECD QSAR Toolbox (LMC, 2013) for (a) mono-alkyldimethylammonium compound with a C_{16} alkyl chain (CAS RN 57-09-0), (b) di-alkyldimethylammonium compound with C_{10} alkyl chains (CAS RN 7173-51-5), and (c) di-alkyldimethylammonium compound with C_{18} alkyl chains (CAS RN 107-64-2):

Taxon	Endpoint	Method
Fish	(a) 96 h LC50 = 0.28 mg/L	Experimental *Oryzias latipes* (Japanese medaka) OECD TG 203

Taxon	Endpoint	Method
	(b) 96 h LC50 = 0.19 mg/L	Experimental *Lepomis macrochirus* (Bluegill)
	(c) 96 h LC50 = 1.04 mg/L	Experimental *Lepomis macrochirus* (Bluegill) Renewal
Invertebrates	(a) 48 h EC50 = 0.016 mg/L	Experimental *Daphnia magna* (Water flea) OECD TG 202
	(b) 48 h LC50 = 0.018 mg/L	Experimental *Daphnia magna* (Water flea) Static
	(c) 48 h LC50 = 0.16 mg/L	Experimental *Daphnia magna* (Water flea)
Algae	(a) 72 h EC50 = 0.0064 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae) OECD TG 201
	(b) 96 h EC50 = 0.014 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae) Static
	(c) 96 h EC50 = 0.46 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae)

While the chemicals in this group also exhibit microbial toxicity, they are not expected to affect wastewater treatment processes at the concentrations found in STPs (Scott and Jones, 2000). Under environmental conditions, microbial populations are expected to be acclimatised to commonly used quaternary ammonium cations (Boethling, 1984; de Oude, 1992).

Chronic toxicity

The following no-observed effect concentration (NOEC) values for model organisms across two trophic levels were reported in the European Union Risk Assessment Report (IHCP, 2009) and the databases included in the OECD QSAR Toolbox (LMC, 2013) for (a) mono-alkyldimethylammonium compound with a C_{16} alkyl chain (CAS RN 57-09-0), (b) di-alkyldimethylammonium compound with C_{10} alkyl chains (CAS RN 7173-51-5), and (c) di-alkyldimethylammonium compound with C_{18} alkyl chains (CAS RN 107-64-2):

Taxon	Endpoint	Method
Invertebrates	(a) 21 d NOEC = 0.023 mg/L	Experimental *Daphnia magna* (Water flea) OECD TG 211
	(b) 21 d NOEC = 0.125 mg/L	Experimental *Daphnia magna* (Water flea)
	(c) 21 d NOEC = 0.38 mg/L	Experimental *Daphnia magna* (Water flea)
Algae	(a) 72 h NOEC = 0.0018 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae) OECD TG 201
	(b) 72 h NOEC = 0.06 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae) OECD TG 201 Read across from di-alkyldimethylammonium chloride with $C_{12\text{-}18}$ alkyl chain
	(c) 96 h NOEC = 0.16 mg/L	Experimental *Pseudokirchneriella subcapitata* (Green algae)

Chronic toxicity information for fish was not available for chemicals in this group.

Effects on Sediment-Dwelling Life

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

The chronic ecotoxicity of mono-alkyl quaternary ammonium compounds with C_{20-22} alkyl chains (CAS RN 68607-24-9) has been investigated for *Lumbriculus variegatus* (Blackworm). A 28 day NOEC of 62.5 µg/g dry weight sediment was obtained for this species following OECD Test Guideline TG 225 (LMC, 2013).

Effects on Terrestrial Life

There are limited soil toxicity data available for chemicals in this group. Some limited reproductive toxicity to earthworms has been observed.

The following NOEC values for terrestrial organisms were reported in the databases included in the OECD QSAR Toolbox (LMC, 2013) for (a) mono-alkyl quaternary ammonium compounds with C_{20-22} alkyl chains (CAS RN 68607-24-9) and (b) di-alkyl quaternary ammonium compounds with C_{10} alkyl chains (CAS RN 7173-51-5):

Taxon	Endpoint	Method
Invertebrate	(a) 54 d NOEC = 250 mg/kg (dry weight) (b) 55 d NOEC = 125 mg/kg (dry weight)	Experimental *Eisenia fetida* (Earthworm) OECD TG 222

Predicted No-Effect Concentration (PNEC)

The aquatic PNECs for two representative chemicals in this group were calculated based on the bioavailable fraction of each chemical estimated to be present in environmental waters.

Laboratory-derived toxicity values in clean test waters overestimate toxicity under environmental conditions as quaternary ammonium surfactants sorb to suspended solids and have a tendency to form complexes with anionic surfactants in natural waters (de Oude, 1992). As a result, the bioavailable fraction of quaternary ammonium surfactants in environmental waters is reduced by up to 95% (Landis, et al., 1993). To correct for this reduction in bioavailability under environmental exposure conditions, the measured ecotoxicity endpoints in laboratory tests can be multiplied by a maximum mitigation factor of 20 (Landis, et al., 1993).

The calculated PNEC for mono-alkyl quaternary ammonium compounds with C_{16} alkyl chains is 3.6 µg/L based on the 72 h NOEC of 0.0018 mg/L for algae. The laboratory endpoint value for algae was divided by an assessment factor of 10 to account for interspecies variation and the derived value was then multiplied by a factor of 20 to account for the 5% bioavailable fraction in environmental waters. The calculated PNEC for di-alkyl quaternary ammonium compounds with C_{10} alkyl chains is 2.8 µg/L based on the 96 h EC50 of 0.014 mg/L for algae. This value was calculated by a similar procedure as applied to the mono-alkyl quaternary ammonium compound, but using an assessment factor of 100 in accordance with standard methodology for deriving PNECs from acute toxicity endpoint values (EPHC, 2009).

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

Toxic (T). Based on available acute ecotoxicity values below 1 mg/L and/or chronic ecotoxicity values below 0.1 mg/L, all chemicals in this group are categorised as Toxic.

Summary

All chemicals in this group are categorised as:

- Not P
- Not B
- T

Risk Characterisation

Based on the PEC and PNEC values determined above, the following Risk Quotients (RQ = PEC ÷ PNEC) have been calculated for the release of two representative chemicals in this group into rivers in treated sewage treatment plant effluent:

Chemical	PEC (µg/L)	PNEC (µg/L)	RQ
hexadecyltrimethylammonium bromide	8.5	3.6	2.4
didecyldimethylammonium chloride	8.5	2.8	3.0

An RQ of greater than one indicates that industrial uses of some mono- and di-alkyl quaternary ammonium compounds may pose an unreasonable risk to the environment, as environmental concentrations may exceed levels that cause harmful effects.

However, it is noted that the RQ values derived using default assumptions (EPHC, 2009; NICNAS, 2013) may be an overestimation of the actual risks. As noted above, the PEC value of 8.5 µg/L is expected to overestimate environmental levels of these chemicals in surface waters in Australia. International monitoring data show total concentrations of mono-alkyl quaternary ammonium compounds with alkyl chain lengths of C_{12-18} in river water up to 1.24 µg/L. If this value is used in place of the PEC for the chemicals in this group, the environmental concentrations of both surfactants in river water will be less than their respective PNECs (i.e., RQ < 1).

Based on this analysis, it is concluded that the RQs calculated for emission of quaternary ammonium surfactants in this group to riverine surface waters are likely to overestimate the risks posed, and that levels of these cationic surfactants in environmental surface waters are therefore unlikely to exceed the level of concern in Australia.

Key Findings

Based on available use and exposure information, chemicals in this group are widely used in a range of products including cleaning and washing agents, cosmetics and biocides. Many of these use patterns have the potential to release these chemicals into sewage treatment plants. While the chemicals in this group can be very toxic to aquatic organisms, they are efficiently removed from wastewater in sewage treatment plants and they typically undergo rapid biodegradation in water and soil.

The concentrations of these chemicals in treated sewage treatment plant effluent released to surface waters are not considered to pose a concern taking into account likely exposure concentrations and considering mitigating factors such as the rapid biodegradation of quaternary ammonium surfactants in the environment, and their relatively low bioavailability in natural environmental waters.

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

Recommendations

The chemicals in this group are not prioritised for further assessment under the IMAP framework.

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) 1-hexadecanaminium, *N*,*N*,*N*-trimethyl-, bromide (CAS RN 57-09-0) and (b) 1-decanaminium, *N*-decyl-*N*,*N*-dimethyl-, chloride (CAS RN 7173-51-5) 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) and (b) Category 1 (H400)	Very toxic to aquatic life
Chronic Aquatic	(a) Category 1 (H410)	Very toxic to aquatic life with long lasting effects
	(b) Category 2 (H411)	Toxic to aquatic life with long lasting effects

The classification of the aquatic hazards posed by these chemicals has been performed based on the toxicity data presented in this assessment. The long-term aquatic hazard classification for both chemicals was determined based on the most stringent outcome method of the GHS taking into account the rapid degradability of these substances and the available chronic ecotoxicity data.

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

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