# Cationic surfactants: Human health tier II assessment

# 03 July 2015

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# **Chemicals in this assessment**

Chemical Name in the Inventory	CAS Number
1-Hexadecanaminium, N,N,N-trimethyl-, bromide	57-09-0
1-Dodecanaminium, N,N,N-trimethyl-, chloride	112-00-5
1-Hexadecanaminium, N,N,N-trimethyl-, chloride	112-02-7
1-Octadecanaminium, N,N,N-trimethyl-, chloride	112-03-8
1-Dodecanaminium, N,N,N-trimethyl-, bromide	1119-94-4
1-Decanaminium, N-decyl-N,N-dimethyl-, chloride	7173-51-5
Quaternary ammonium compounds, alkylbenzyldimethyl, chlorides	8001-54-5
1-Docosanaminium, N,N,N-trimethyl-, chloride	17301-53-0
Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides	61789-71-7



Chemical Name in the Inventory	CAS Number
Quaternary ammonium compounds, benzyl-C8- 18-alkyldimethyl, chlorides	63449-41-2
Quaternary ammonium compounds, benzyl- C12-18-alkyldimethyl,chlorides	68391-01-5
Quaternary ammonium compounds, benzyl- C12-16-alkyldimethyl,chlorides	68424-85-1
Quaternary ammonium compounds, benzyl- C12-18-alkyldimethyl,salts with 1,2- benzisothiazol-3(2H)-one 1,1-dioxide (1:1)	68989-01-5
Quaternary ammonium compounds, benzyl- C12-14-alkyldimethyl,chlorides	85409-22-9

# **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

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#### **ACRONYMS & ABBREVIATIONS**

# **Grouping Rationale**

The chemicals in this category are basically soaps or detergents and are comprised of 14 separate quaternary ammonium compounds, with their hydrophilic end being a cationic quaternary ammonium group, with chloride or bromide counterions. This category is based on the structural and functional similarities of cationic surfactants and their similar physicochemical properties, biodegradability, aquatic toxicity and environmental disposition patterns. A similar hazard profile for human health is also expected.

The chemicals in this group have similar reported uses.

# Import, Manufacture and Use

#### **Australian**

The following Australian industrial uses were reported under previous mandatory and/or voluntary calls for information for C12–18 alkyl dimethyl benzyl ammonium chloride (CAS No. 68391-01-5), C12–16 alkyldimethylbenzylammonium chloride (CAS No. 68424-85-1), and benzyl C12-14 alkyldimethylammonium chloride (CAS No. 85409-22-9).

The chemicals have reported domestic use including in cleaning and washing agents, and additives.

The total volume introduced into Australia, reported under previous mandatory and/or voluntary calls for information, was between 100 and 1000 tonnes for the above stated two chemicals (CAS Nos. 68391-01-5, 68424-85-1, 85409-22-9).

Dodecyltrimethylammonium bromide (CAS No. 1119-94-4) has reported commercial use in automotive coatings.

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

#### International

The following international uses have been identified through European Union Registration, Evaluation, Authorisation and Restriction of Chemicals (EU REACH) dossiers; the Organisation for Economic Cooperation and Development Screening Information Dataset Initial Assessment Report (OECD SIAR); Galleria Chemica; Substances and Preparations in the Nordic countries (SPIN) database; the European Commission Cosmetic Ingredients and Substances (CosIng) database; United States (US) Personal Care Product Council International Nomenclature of Cosmetic Ingredients (INCI) dictionary; and eChemPortal: OECD High Production Volume chemical program (OECD HPV), the US Environmental Protection Agency's Aggregated Computational Toxicology Resource (ACToR), and the US National Library of Medicine's Hazardous Substances Data Bank (HSDB).

The majority of chemicals in this group have reported cosmetic use including:

- as preservative and antimicrobial agents;
- as surfactant, antistatic, and emulsifying agents; and
- in hair conditioner and deodorant/perfumes.

Some chemicals in this group have reported cosmetic uses in the US (Personal Care Products Council, 2011). These chemicals are cetrimonium bromide (CAS No. 57-09-0), dodecyltrimethylammonium chloride (CAS No. 112-00-5), cetrimonium chloride (CAS No. 112-02-7), stearyl trimethyl ammonium chloride (CAS No. 112-03-8), didecyl dimethyl ammonium chloride (CAS No. 7173-51-5), benzalkonium chloride (CAS No. 8001-54-5), behentrimonium chloride (CAS No. 17301-53-0), C12-18 alkyl dimethyl benzyl ammonium chloride (CAS No. 68391-01-5), and myristalkonium saccharinate (CAS No. 68989-01-5).

Some chemicals in this group have reported domestic use including in:

	adhesives	(binding	agents)	and	fillers;
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- cleaning/washing agents;
- colouring agents;
- odour agents;
- corrosion inhibitors;
- paints, lacquers and varnishes;
- surface treatment;
- surface-active agents; and
- germicides and fungicides.

The US Household Products Database states a concentration of up to: <5 % (liquid) of didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) for home maintenance use; 0.145 % (wipes) and 0.15 % (sheets) of cocodimethyl benzyl ammonium chloride (CAS No. 61789-71-7) for inside the home and personal care uses, respectively; 5 % (liquid) of alkyl dimethyl benzyl ammonium chloride (CAS No. 63449-41-2) for inside the home use; 32 % (liquid) of C12–18 alkyl dimethyl benzyl ammonium chloride (CAS No. 68391-01-5) for landscape use; and 1 % and 2.4 % (liquid) of C12–16 alkyldimethylbenzylammonium chloride (CAS No. 68424-85-1) for personal care and inside the home uses, respectively; and up to 1 % (aerosol) of myristalkonium saccharinate (CAS No. 68989-01-5) for inside the home use.

Some chemicals in this group have reported commercial use including in:

- absorbents and adsorbents;
- conductive agents;
- construction materials and in cutting fluids;
- lubricants and additives;
- impregnation materials;
- process regulators and softeners;
- surface active agents; and
- anti-freezing agents.

Some chemicals in this group have reported site-limited use including in:

- laboratory reagents; and
- electroplating agents.

The following non-industrial uses have been identified internationally for some chemicals in this group including:

- in pharmaceutical preparations (topical antiseptic/disinfectant);
- in non-agricultural pesticides and preservatives;

- in agricultural pesticides; and
- as antimicrobial chemicals with germicidal, fungicidal and algicidal activity.

# Restrictions

#### **Australian**

Quaternary ammonium compounds are listed in the *Poisons Standard* (Standard for the Uniform Scheduling of Medicines and Poisons (SUSMP, 2013)) in Schedule 5 as follows:

'QUATERNARY AMMONIUM COMPOUNDS in preparations containing 20 per cent or less of quaternary ammonium compounds **except**:

- (a) when separately specified in these Schedules;
- (b) dialkyl or dialkoyl quaternary ammonium compounds where the alkyl or alkoyl groups are derived from tallow or hydrogenated tallow or similar chain length (C16/C18) sources; or
- (c) in preparations containing 5 per cent or less of such quaternary ammonium compounds'.

Quaternary ammonium compounds are also listed in the Poisons Standard (SUSMP, 2013) in Schedule 6 as follows:

#### 'QUATERNARY AMMONIUM COMPOUNDS except:

- (a) when separately specified in these Schedules;
- (b) when included in Schedule 5;
- (c) dialkyl or dialkoyl quaternary ammonium compounds where the alkyl or alkoyl groups are derived from tallow or hydrogenated tallow or similar chain length (C16/C18) sources; or
- (d) in preparations containing 5 per cent or less of such quaternary ammonium compounds'.

Benzalkonium chloride (CAS No. 8001-54-5) is listed in the Poisons Standard (SUSMP, 2013) in Schedule 5 as follows:

'BENZALKONIUM CHLORIDE in preparations containing 10 per cent or less of benzalkonium chloride **except** in preparations containing 5 per cent or less of benzalkonium chloride'.

Benzalkonium chloride (CAS No. 8001-54-5) is also listed in the Poisons Standard (SUSMP, 2013) in Schedule 6 as follows:

#### 'BENZALKONIUM CHLORIDE except:

- (a) when included in Schedule 5; or
- (b) in preparations containing 5 per cent or less of benzalkonium chloride'.

Schedule 6 chemicals are labelled with 'Poison'. These are substances with a moderate potential for causing harm, the extent of which can be reduced by using distinctive packaging with strong warnings and safety directions on the label.

Schedule 5 chemicals are labelled with 'Caution'. These are substances with a low potential for causing harm, the extent of which can be reduced through the use of appropriate packaging with simple warnings and safety directions on the label.

#### International

The chemicals in this group are listed on the following (Galleria Chemica).

Some chemicals in this group (CAS Nos. 57-09-0, 112-00-5, 112-02-7, 112-03-8, 1119-94-4, 68989-01-5) are listed on EU Cosmetics Regulation 1223/2009 Annex V—List of preservatives allowed in cosmetic products—with a maximum concentration allowed in ready-for-use preparations being 0.1 %. These chemicals are also listed on the *New Zealand cosmetic products group standard*—Schedule 7: List of preservatives allowed—with a maximum authorised concentration being 0.1 %.

Some chemicals in this group (CAS Nos. 112-02-7, 112-03-8) are listed on EU Cosmetics Regulation 1223/2009 Annex III—List of preservatives allowed in cosmetic products—with a maximum concentration allowed in rinse-off hair products being 2.5 %, in leave-on hair products being 1 %, and in leave-on face products being 0.5 %.

In addition, benzalkonium chloride, bromide and saccharinate (CAS No. 63449-41-2) is also listed on: EU Cosmetic Regulation 1223/2009 Annex III—List of substances which cosmetic products must not contain except subject to the restrictions—with a maximum authorised concentration in the finished cosmetic product of 3 % for 'Rinse-off (head) care' products; and New Zealand Cosmetic Products Group Standard—Schedule 5: Components cosmetic products must not contain except subject to the restrictions: Maximum authorised concentration in the finished cosmetic product is 3 % for 'Rinse-off (head) care' products and 0.1 % for other products. Further, the concentration of benzalkonium chloride, bromide and saccharinate with an alkyl chain of C14 or less must not exceed 0.1 % in the final product.

One chemical of this group, benzyl C12-14 alkyldimethylammonium chloride (CAS No. 85409-22-9), is listed on the following (Galleria Chemica):

Health Canada List of prohibited and restricted cosmetic ingredients (The Cosmetic Ingredient "Hotlist").

# **Existing Worker Health and Safety Controls**

#### **Hazard Classification**

Didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) and alkyl dimethyl benzyl ammonium chloride (CAS No. 63449-41-2) are classified as hazardous, with the following risk phrases for human health in the Hazardous Substances Information System (HSIS) (Safe Work Australia):

- Xn; R22 (Acute toxicity)
- C; R34 (Corrosive)

In addition, the following risk phrase for human health is also noted for alkyl dimethyl benzyl ammonium chloride (CAS No. 63449-41-2) in the HSIS (Safe Work Australia): Xn; R21 (Acute toxicity)

# **Exposure Standards**

#### Australian

No specific exposure standards are available for chemicals in this group.

International

No specific exposure standards are available for chemicals in this group.

# **Health Hazard Information**

# **Toxicokinetics**

Although limited data are available for specific chemicals in this group, quaternary ammonium compounds are poorly absorbed through the oral exposure. Dermal absorption is also very low and systemic effects from percutaneous absorption through intact skin are rare. However, dermal absorption can occur through damaged skin (IPCS, 1999; REACHa).

The chemical cetrimonium bromide (CAS No. 57-09-0) was indicated to be poorly absorbed in the gastro-intestinal tract in rats following oral administration. Total excretion in faeces was 92 % and in urine 1 % of the administered dose after three days. It was also indicated that the chemical was not preferentially distributed to any single target organ (REACHa).

# **Acute Toxicity**

#### Oral

The chemicals in this group have moderate acute toxicity following oral exposure in animal tests. While the appropriate data are limited for some members of this group, information was sufficiently available across the group to support classification (refer to **Recommendation** section).

Two members of this group, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) and alkyl dimethyl benzyl ammonium chloride (CAS No. 63449-41-2), are classified as hazardous with the risk phrase 'Harmful if swallowed' (Xn; R22) in the Hazardous Substances Information System (HSIS) (Safe Work Australia).

The reported oral median lethal dose (LD50) in rats was 410 mg/kg bw for cetrimonium bromide (CAS No. 57-09-0), 490–560 mg/kg bw for dodecyltrimethylammonium chloride (CAS No. 112-00-5), 400–600 mg/kg bw for cetrimonium chloride (CAS No. 112-02-7), 536–633 mg/kg bw for stearyl trimethyl ammonium chloride (CAS No. 112-03-8), 238–262 mg/kg bw for didecyl dimethyl ammonium chloride (CAS No. 7173-51-5), and 280–305 mg/kg bw for benzalkonium chloride (CAS No. 8001-54-5). Observed sub-lethal effects included sluggishness, lacrimation, diarrhoea, ataxia, loss of righting reflex, red stains around the nose and mouth, and brown stains on the periurogenital fur (IPCS, 1999; US EPA 2006, 2008; SCCS, 2009; Consumer Specialty Products Association, 2011; REACHa-e; RTECS).

#### Dermal

The chemicals in this group are likely to have low to moderate acute dermal toxicity in animal tests. While the appropriate data are limited for some members of this group, information was sufficiently available across the group to support classification (refer to **Recommendation** section). It is noted that, as chemicals in this group are poorly absorbed through intact skin following dermal exposure (see **Toxicokinetics**), the observed lethality is not likely as a result of systemic toxicity through percutaneously absorbed material. Although the association was not clearly demonstrated here, the dermal LD50 values across this group are likely to show dependency on the concentration at which the chemicals are applied, consistent with toxicity due to local tissue damage. On this basis, all chemicals in this group should be considered harmful if applied at corrosive concentrations (US EPA, 2008; SCCS, 2009; Consumer Specialty Products Association, 2011; HSDB; REACHa—e; RTECS).

One member of this group, alkyl dimethyl benzyl ammonium chloride (CAS No. 63449-41-2), is classified as hazardous with the risk phrase 'Harmful in contact with the skin' (Xn; R21) in the Hazardous Substances Information System (HSIS) (Safe Work Australia).

The reported dermal median lethal dose (LD50) in rats was 4300 mg/kg bw for cetrimonium chloride (CAS No. 112-02-7) (undiluted); >2930 mg/kg bw (65 % purity) and >1000 mg/kg bw (undiluted) for didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) (65 % purity); 930 mg/kg bw for benzalkonium chloride (CAS No. 8001-54-5) (82.26 % purity); 1420 mg/kg bw for C8–18-alkydimethylbenzyl ammonium chlorides (CAS No. 63449-41-2) (undiluted); 2300 mg/kg bw for C12–18 alkyl dimethyl benzyl ammonium chloride (CAS No. 68391-01-5) (undiluted); and 2848 mg/kg bw for C12–16 alkyldimethylbenzylammonium chloride (CAS No. 68424-85-1) (undiluted). A value of 528 mg/kg bw (undiluted) has also been reported for cetrimonium chloride (CAS No. 112-02-7) and for stearyl trimethyl ammonium chloride (CAS No. 112-03-8) as a read across from coconut alkyltrimethyl chlorides (CAS No. 61789-18-2). Observed sub-lethal effects included somnolence (generally depressed activity), dermatitis, and haemorrhages.

Information on acute dermal toxicity was not available on some members of this group such as cetrimonium bromide (CAS No. 57-09-0), dodecyltrimethylammonium chloride (CAS No. 112-00-5), laurtrimonium bromide CAS No. 1119-94-4), behentrimonium

chloride (CAS No. 17301-53-0), alkyl dimethyl benzyl ammonium chloride (CAS No. 61789-71-7), benzyl C12-14-alkyldimethylammonium chloride (CAS No. 65409-22-9), and myristalkonium saccharinate (CAS No. 68989-01-5).

Inhalation

No data are available.

#### Observation in humans

Although data are not available on children, fatalities in adult humans have been reported following an oral dose of 100–400 mg/kg bw or a parenteral dose of 5–15 mg/kg bw of quaternary ammonium compounds. Other signs of poisoning may include nausea, vomiting, abdominal pain, anxiety, restlessness, coma, convulsions, hypotension, cyanosis, and apnoea due to respiratory muscle paralysis. Death can occur within one or three hours after ingestion of concentrated solutions. Haemolysis and methaemoglobinaemia have been reported infrequently (IPCS, 1999).

Following ingestion of higher concentrations of benzalkonium chloride (CAS No. 8001-54-5), mild to severe caustic burns on the lips, tongue, mouth, throat, hypopharynx, oesophagus, and stomach can occur; hypersalivation, vomiting, haematemesis, diarrhoea and confusion can also occur. In severe cases, there could be hypotension, shock, respiratory paralysis, convulsions, coma, and cardiorespiratory arrest. Intravenous and intrauterine administration of quaternary ammonium compounds can cause haemolysis (IPCS, 1999).

Benzalkonium chloride (CAS No. 8001-54-5) at 11 % concentration, instead of 1:50000 dilution, was mistakenly given orally to two-and-a-half-month-old twins for candidiasis. Both children developed irritability, fever, anorexia, dehydration, cough, circumoral erythema, drooling and numerous oral and pharyngeal lesions within 24 hours. In addition, one twin also developed chemical pneumonitis (IPCS, 1999).

#### **Corrosion / Irritation**

# Corrosivity

Chemicals in this group are considered to be corrosive chemicals. While the appropriate data are limited for some members in this group, information on application of high concentration solutions was sufficiently available across the group in animals and humans to support classification (refer to **Recommendation** section) (IPCS, 1999; US EPA, 2008; SCCS, 2009; REACHb–d).

Two members in this group, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) and alkyl dimethyl benzyl ammonium chloride (CAS No. 63449-41-2), are classified as hazardous, with the following risk phrase for human health in the Hazardous Substances Information System (HSIS) (Safe Work Australia) 'C; R34 (Corrosive)'.

In an acute dermal irritation study conducted according to OECD Test Guideline (TG) 404, stearyl trimethyl ammonium chloride (CAS No. 112-03-8) at 79.8 % concentration was applied on the clipped dorsal area of four New Zealand White rabbits. While three animals were exposed for only three minutes, one animal was exposed for four hours. Signs of irritation were not noted following exposure for three minutes. However, very slight to well-defined erythema and very slight oedema were seen from 30–60 minutes up to 22 days following the four-hour exposure. During the observation period, the treated skin was sporadically dry, rough, indurated, encrusted, chapped and discoloured beige. Pink coloured new skin and scarring was noted following 22 days of application. The chemical was therefore considered to be corrosive to the skin (SCCS, 2009; REACHc).

In another acute dermal irritation study conducted according to OECD TG 404, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) at 52 % concentration was applied on the clipped dorsal area of six New Zealand White rabbits. While three animals were exposed for only three minutes, the other three animals were exposed for four hours. In the three-minute exposure group, slight erythema and slight to severe oedema was noted up to seven days after application. At the end of the 14-day observation period, the skin appeared dry, rough, and leather-like. The mean score for oedema and erythema was 4 in observations up to 72 hours. In the four-hour exposure group, severe erythema and severe oedema was noted up to 72 hours after application and the skin appeared rough, dry and scabbed with discoloration. All animals in the four-hour exposure group were euthenised after the 72-hour observation period. The chemical was therefore considered to be corrosive to the skin.

In another acute dermal irritation study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) at 80 % concentration was considered to be corrosive to the skin in six New Zealand White rabbits. While three animals were exposed for only three minutes, the other three animals were exposed for one hour. Following the one hour exposure, skin lesions noted at the treated skin sites were light brown discoloration of the epidermis and slight haemorrhage of the dermal capillaries; eschar had developed at all treated skin sites at 24 hours after exposure and continued to be present at the 48 and 72 hour, and at day seven observations. Blanching and moderate erythema were also noted during this period and sunken eschar was noted at all the treated skin sites on day 14 (REACHd).

In another study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) (80 % concentration) was applied to the skin of one rabbit. This study was terminated after 24 hours due to corrosion. Changes noted in the coloration and/or texture of the skin included coriaceousness (leather-like), blanching, green/brown discoloration, brown/dark red discoloration, and necrosis (US EPA, 2008).

In an acute dermal irritation study, conducted similar to OECD TG 404, 24–26 % and 28–30 % cetrimonium chloride (CAS No. 112-02-7) were applied to the intact skin of three New Zealand White rabbits for four hours. The mean score values of 24–26 % cetrimonium chloride (CAS No. 112-02-7) at the 24-, 48- and 72-hour post application readings were 3 for erythema and 1.9 for oedema. At days seven and 14, grade 2–3 erythema and grade 1–2 oedema were found. At day 14, oedema was observed only in one animal. The mean score values of 28–30 % cetrimonium chloride (CAS No. 112-02-7) at the 24-, 48- and 72-hour readings were 2.9 for erythema and 1.6 for oedema. At days seven and 14, oedema was not noted but grade two erythema was found. At day 21, adverse skin reactions were absent. The chemical was therefore considered to be a moderate skin irritant at the stated concentrations (SCCS, 2009; REACHb).

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No data are available.

#### Eye Irritation

Although data are limited, chemicals in this group are considered to be corrosive chemicals. Corrosive chemicals are also considered to cause irreversible effects on the eyes; the available eye irritation data for chemicals in this group support this finding (US EPA, 2008; SCCS, 2009; REACHb).

In an acute eye irritation study conducted similarly to OECD TG 405, 24–26 % and 28–30 % cetrimonium chloride (CAS No. 112-02-7) were placed into the conjunctival sac of one eye of each of three New Zealand White rabbits. The mean score values of 24–26 % cetrimonium chloride (CAS No. 112-02-7) at the 24, 48 and 72 hour readings after exposure were 2.8 for corneal opacity, 2.4 for conjunctival redness and 4.0 for conjunctival chemosis. Corneal opacity and conjunctival irritation (evident as redness and swelling) persisted until day 21. The mean score values of 28–30 % cetrimonium chloride (CAS No. 112-02-7) at the 24, 48 and 72 hour readings were 1.9 for corneal opacity, 1.0 for iritis, 2.3 for conjunctival redness and 3.7 for conjunctival chemosis. Corneal opacity and conjunctival irritation (as grade 1–2 redness) and swelling (grade 2) also persisted until day 21. As the eye lesions persisted until day 21, the chemical was considered to cause irreversible eye damage (REACHb; SCCS, 2009).

In another eye irritation study conducted according to the US Federal guideline (16 CFR 1500.42), 0.1 ml of a 5 % cetrimonium chloride (CAS No. 112-02-7) solution was placed into the conjunctival sac of one eye of six New Zealand White rabbits. The ocular lesions were evaluated according to the Draize method and were further classified by the modified method of Kay and Calandra. All treated eyes had corneal opacity, iritis and conjunctival irritation during the 24 to 72 hour test period. The maximum mean total scores of 53, 60, and 58 were noted at 24, 48, and 72 hours, respectively. Based on these scores, the chemical was considered to be highly irritating at a 5 % concentration (REACHb).

In an acute eye irritation study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) (80 % concentration) was instilled into the eye of one male rabbit for one hour. The chemical produced extreme corneal opacity, iritis and conjunctival irritation observed one hour following exposure. The eye also appeared to be misshapen. The total irritation score for the single animal was determined to be 94 out of a maximum of 110 one hour following exposure. As corrosion was exhibited at this time, the study was terminated at this point, without testing additional animals (US EPA, 2008).

# Observation in humans

The chemicals in this group can cause mild to severe caustic burns of the skin and mucous membranes, depending on the chemical involved and the concentration. Benzalkonium chloride (CAS No. 8001-54-5) has been reported to be a human skin and severe eye irritant, and caustic actions have been reported with diluted solutions (1:2000, 1:5000, 1:20000). Accidental spillage of concentrated solution of benzalkonium chloride (CAS No. 8001-54-5) on the skin can produce corrosive skin lesions with deep necrosis and scarring (IPCS, 1999; HSDB).

While a diluted solution (0.1 % concentration) of benzalkonium chloride (CAS No. 8001-54-5) might only result in mild discomfort to the eyes, a concentrated solution of 10 % can cause very serious corneal damage. Intranasal administration of 0.5–0.10 % of benzalkonium chloride (CAS No. 8001-54-5) in rats has caused nasal lesions (HSDB; IPCS, 1999). The primary dermal effects that have been reported following exposure to quaternary ammonium compounds are rashes, burning sensation, numbness, and itching. Nausea, headache, and sore throat have been reported as the primary systemic effects (HSDB).

In epicutaneous patch tests, 2.5 % and 3.5 % cetrimonium chloride (CAS No. 112-02-7) were applied to the backs of human volunteers for one hour, and to the ventral side of the forearm of human volunteers using Finn chambers for 24 hours. The skin reactions were evaluated at 15 minutes and at 24 and 48 hours after exposure. It was concluded that while 2.5 % cetrimonium chloride in a cosmetic formulation caused some skin irritation, 3.5% cetrimonium chloride in a cosmetic formulation caused slight to moderate skin irritation (REACH).

The quaternary ammonium compounds were responsible for extensive inner ear destruction in guinea pigs following a shorter period of middle ear exposure (IPCS, 1999).

The California Department of Pesticide Regulation (1982–2004) has recorded incidents associated with exposure to end-use products containing quaternary ammonium compounds. While incidents involving oral exposure resulted in irritation to the mouth/throat/nose, vomiting/nausea/abdominal pain, dizziness, and headache; incidents involving inhalation exposure resulted in respiratory irritation/burning, irritation to the mouth/throat/nose, coughing/choking, chest pain, disorientation, dizziness, and shortness of breath. Irritation/burning, rash, itching and blistering were noted during incidental dermal exposure. Hives and allergic contact dermatitis were also noted following dermal exposure. Incidental exposure of eyes resulted in irritation/burning, eye pain, conjunctivitis, eye, and eyelid swelling (HSDB).

#### Sensitisation

#### Skin Sensitisation

Although limited information is available on the skin sensitisation potential of these chemicals, based on the available information, the chemicals in this group are not likely to be skin sensitisers. Considering many years' use of these chemicals, some rare clinical reports of skin sensitisation are considered to be of little relevance (IPCS, 1999; US EPA, 2008; SCCS, 2009; REACHc-d).

In a skin sensitisation study conducted according to OECD TG 406 (Buehler test) in Pirbright-White guinea pigs, animals were exposed to 0.5 mL of the cetrimonium chloride (CAS No. 112-02-7) at 4 % w/v for six hours during the induction phase on the shaved skin of the left flank. During the challenge phase (day 29), animals were exposed to 0.5 mL of the chemicals at 1 % on the shaved skin of the right flank. While animals presented light to clearly defined erythema and very light oedema during the induction phase, no effects were observed in any animals of the treated group following the challenge. The chemical was therefore not considered to be skin sensitising (SCCS, 2009; REACHb). Cetrimonium chloride (CAS No. 112-02-7) was also negative in a guinea pig skin maximisation test with induction at 0.125 % concentration and challenge at 0.5 % concentration (SCCS, 2009; REACHb). In another skin sensitisation study conducted according to OECD TG 406 (Buehler test) in Pirbright-White guinea pigs, stearyl trimethyl ammonium chloride (CAS No. 112-03-8) at induction and challenge doses of 4 and 1 %, respectively, was not considered to be a skin sensitiser (SCCS, 2009; REACHc).

In another skin sensitisation study conducted according to OECD TG 406 (Buehler test), Dunkin-Hartley guinea pigs were repeatedly induced with didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) at 2 % for six hours on the shaved skin of the left flank. Animals were then challenged with the chemical at 1 % concentration 14 days later (day 29). Slight to severe oedema, well-defined to severe erythema, and necrotic areas were observed in the treated skin of experimental animals after the third topical induction exposure (day 15) but no responses were seen at challenge. The chemical was not considered to have sensitisation potential (REACHd).

In another skin sensitisation study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was topically administered to guinea pigs at 0.25, 0.5 or 0.75 % once a week for three weeks during the induction phase. Animals were then challenged with the chemical at 0.1 % concentration over 27 days. No positive responses were noted in any of the test animals (US EPA, 2008).

#### Observation in humans

There have been reports of irritant contact dermatitis in humans following exposure to quaternary ammonium compounds, particularly benzalkonium chloride (CAS No. 8001-54-5). Allergic conjunctivitis has been reported in two physicians from handling the instruments soaked in the disinfectant solution containing benzalkonium chloride (CAS No. 8001-54-5) for cold sterilisation (IPCS, 1999; HSDB).

#### **Repeated Dose Toxicity**

#### Oral

Although the appropriate data are limited, the chemicals in this group are not considered to cause serious damage to health from repeated oral exposure at doses below acutely toxic doses. Lesions have been noted in these studies, possibly due to the corrosive nature of these chemicals having direct effects to the gastrointestinal tract (US EPA, 2008; SCCS, 2009; Consumer Specialty Products Association 2011; REACHa—b).

Several repeated dose oral toxicity studies have been conducted on chemicals in this group. As stated above, observed effects were mainly due to the direct irritant effects of these chemicals to the gastrointestinal tract and included decreased body weight and weight gain; increased adrenal and liver weights; increased histiocytic hyperplasia in the mesenteric lymph nodes; and lesions in the gastrointestinal tract.

In a repeated dose oral toxicity study, cetrimonium bromide (CAS No. 57-09-0) was administered orally to Sprague Dawley (SD) rats (10/sex/dose) at 10, 20, and 45 mg/kg bw/day for one year. While significantly reduced mean body weights and reduced skeletal growth (judged by the growth of the tail) were observed in both sexes at the highest tested dose, significantly decreased efficiency of food conversion was noted only in males at the highest tested dose. Relative caecum weight was increased in males at 20 mg/kg bw/day and in both sexes at 45 mg/kg bw/day. No macroscopic or microscopic alterations were found in the stomach wall and small intestine of treated rats. It was suggested that continued administration of the chemical in large doses could have prevented proper nutrition by increasing the rate of gastric emptying and intestinal transit and/or by interfering with the absorption of nutritional substances. A no observed adverse effect level (NOAEL) of 10 mg/kg bw/day was determined (SCCS, 2009; REACHa).

In another repeated dose oral toxicity study, cetrimonium chloride (CAS No. 112-02-7) was administered (gavage) to SD rats at 0, 30, 100, and 300 mg/kg bw/day for 28 days. Inflammatory oedema of the forestomach mucosa, sporadic ulceration, and acanthosis up to papillomatous hyperplasia in both sexes were noted at the highest tested dose of 300 mg/kg bw/day. It was concluded that these changes can be considered a result of local irritation and therefore are not indicative of systemic toxicity. The NOAEL for systemic effects was determined to be 300 mg/kg bw/day (highest tested dose) (SCCS, 2009; REACHb).

In a repeated dose oral toxicity study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was administered to rats (10/sex/dose) in the diet at 0, 6.2, 18.5, 36.8, 60.7 and 175.4 mg/kg bw/day for males and 0, 7.5, 22.3, 44.4, 74.3 and 225.5 mg/kg bw/day for females for 13 weeks. High-dose animals showed increased mortality; decreased mean body weights, body weight gain, and food consumption; and increased incidence of gross pathological observations and non-neoplastic lesions, including higher incidence of glycogen depletion in the liver and contracted spleens. Sinus erythrocytosis and lymphoid hyperplasia of mesenteric lymph nodes were also noted in high-dose females. The NOAEL was established as 60.7 mg/kg bw/day and 74.3 mg/kg bw/day in males and females, respectively, based on increased mortality and effects on body weights, liver and spleen at the next highest dose.

In another combined chronic toxicity/carcinogenicity study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was administered to SD rats (60/sex/dose) in the diet at approximately 0, 13, 32 or 64 mg/kg bw/day for males and 0, 16, 41 or 83 mg/kg bw/day for females for two years (see **Carcinogenicity**). Treatment-related effects in the high-dose animals included decreased mean body weight, increased incidence of sinusoidal blood, haemosiderosis, and histiocytosis in the mesenteric lymph nodes (US EPA, 2008).

In a repeated dose oral toxicity study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was administered to CD-1 mice (60/sex/dose) in the diet at 0, 100, 500 or 1000 ppm (approximately 0, 15.0, 76.3 or 155.5 mg/kg bw day for males and 0, 18.6, 93.1 or 193.1 mg/kg bw/day for females) for 78 weeks. Decreased mean body weights and body weight gains were the only treatment-related effects noted at the highest tested dose. The NOAEL was established as 76.3/93.1 mg/kg bw/day for males/females (US EPA, 2008).

#### Dermal

As dermal absorption is very low, systemic effects from percutaneous absorption through intact skin are not likely. However, dermal absorption can occur through damaged skin and a range of dermal effects such as erythema, oedema, atonia, and desquamation have been noted at the treatment sites following repeated dermal application (see **Toxicokinetics**).

In a repeated dose dermal toxicity study, cetrimonium chloride (CAS No. 112-02-7) was applied to the abraded skin of New Zealand White rabbits (5/sex/dose) at 0 and 10 mg/kg bw/day for 6.5–7 hours/day, five days/week for 28 days. There were no treatment-related effects on body weight, haematology, organ weight, gross necropsy or histopathology (except for treated areas of the skin). Erythema (slight to moderate) and fissuring at the areas of dermal application were the only signs of dermal irritation noted in all rabbits at 10 mg/kg bw/day and subsided after day 17. A NOAEL of >10 mg/kg bw/day, based on no systemic effects at the only tested dose, was established (REACHb; SCCS, 2009; US EPA, 2008).

In another repeated dose dermal toxicity study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was applied dermally to SD rats (15/sex/dose) at 0, 2, 6 and 12 mg/kg bw/day for six hours/day, five days/week for 13 weeks. Treatment-related systemic effects were not noted and effects were only limited to areas of treated skin of females at 6 mg/kg bw/day and that of males and females at 12 mg/kg bw/day. Gross findings of erythema, oedema, exfoliation, excoriation, and ulceration were also confirmed by histopathological examination; increased incidence of hyperkeratosis, acanthosis, dermatitis, and ulceration were only noted after five days of exposure. As systemic effects were not observed in the study, the NOAEL for systemic effects was established as 12 mg/kg bw/day (highest tested dose). The NOAEL for dermal effects was reported as 2 mg/kg bw/day (US EPA, 2008).

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No data are available.

# Genotoxicity

Although the appropriate data are limited for chemicals in this group, the available information indicate that the chemicals in this group are not considered to have mutagenic or genotoxic potential (US EPA, 2008; IPCS, 2009; SCCS, 2009; Consumer Specialty Products Association 2011; REACHa—e).

Dodecyltrimethylammonium chloride (CAS No. 112-00-5), cetrimonium chloride (CAS No. 112-02-7), stearyl trimethyl ammonium chloride (CAS No. 112-03-8), and didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) were not mutagenic in bacterial reverse mutation assays. Dodecyltrimethylammonium chloride (CAS No. 112-00-5) was also not mutagenic in mouse lymphoma L5178Ycells.

Cetrimonium chloride (CAS No. 112-02-7) and didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) did not induce chromosomal aberrations in V79 Chinese hamster cells and Chinese hamster ovary cells, respectively.

Dodecyltrimethylammonium chloride (CAS No. 112-00-5) and didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) were not mutagenic in an unscheduled DNA synthesis (UDS) assay using rat primary hepatocytes.

Dodecyltrimethylammonium chloride (CAS No. 112-00-5) failed to induce chromosomal aberrations in a bone marrow cytogenetic assay in rats.

# Carcinogenicity

Limited data are available on chemicals in this group and carcinogenicity information was available only on one chemical in this group. The chemicals in this group are also considered not to have mutagenic or genotoxic potential (see **Genotoxicity**). Therefore, it is considered unlikely that the chemicals in this group will have carcinogenic potential.

In a combined chronic toxicity/carcinogenicity study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was administered to SD rats (60/sex/dose) in the diet at approximately 0, 13, 32 or 64 mg/kg bw/day for males and 0, 16, 41 or 83 mg/kg bw/day for females for two years (see **Repeat dose toxicity: oral**). Even though the maximum tolerated dose was achieved in this study for carcinogenicity testing (based on a slight, but statistically significant, decrease in mean body weight and some histopathological changes), there was no evidence of carcinogenicity in this study. In a similar study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5 was administered to CD-1 mice (60/sex/dose) in the diet at approximately 0, 15.0, 76.3 or 155.5 mg/kg bw/day for males and 0, 18.6, 93.1 or 193.1 mg/kg bw/day for females for 78 weeks. Treatment-related mortality or clinical signs, and gross and histopathological abnormalities were not observed. There was also no evidence of carcinogenicity (US EPA, 2008).

Carcinogenicity was also not seen in another study where SD rats were fed didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) at 12.6, 27.3 and 55.4 mg/kg bw/day for males and 15.7, 33.8 and 69.5 mg/kg bw/day for females for 104 weeks (REACHd).

# **Reproductive and Developmental Toxicity**

Although the appropriate data are limited, chemicals in this group are not considered to have specific reproductive or developmental toxicity. Any reproductive and developmental effects were only observed secondary to maternal toxicity. This is also supported by the findings that quaternary ammonium compounds are poorly absorbed through oral exposure (see **Toxicokinetics**).

In a developmental toxicity study, dodecyltrimethylammonium chloride (CAS No. 112-00-5) was administered (gavage) to pregnant New Zealand White rabbits (13/dose) at 0, 2, 8 and 24 mg/kg bw/day from gestation days (GD) 6–18. As no maternal, developmental or foetal treatment-related effects were observed at any tested dose, the NOAEL was determined to be 24 mg/kg bw/day (US EPA, 2008).

In another developmental toxicity study, pregnant New Zealand White rabbits (16/dose) were administered didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) by gavage at 0, 1, 3 and 10 mg/kg bw/day from GD 6–18. At the mid and high doses, maternal toxicity was evident as hypoactivity, laboured and/or audible respiration and decreased body weight gain. An increased maternal mortality was noted at 10 mg/kg bw/day. Developmental effects included increased incidences of foetal mortality and reduced foetal body weight per litter at 10 mg/kg bw/day. The NOAEL for maternal toxicity was established as 1 mg/kg bw/day, based on reductions in body weight gain, hypoactivity, laboured/audible respiration, and mortality. The NOAEL for developmental toxicity was established as 3 mg/kg bw/day, based on increased mortality, decreased foetal body weight, and an increased number of dead foetuses.

In another developmental toxicity study, didecyl dimethyl ammonium chloride (CAS No. 7173-51-5) was administered to pregnant SD rats (25/dose) by gavage at doses of 0, 1, 10 and 20 mg/kg bw/day on GD 6–15. The NOAEL for maternal toxicity was established as 1 mg/kg bw/day, based on decreased body weight gain, low food efficiency, and audible respiration. The NOAEL for developmental toxicity was established as 10 mg/kg bw/day, based on an increased incidence of skeletal variations at the next higher dose (US EPA, 2008).

In a developmental toxicity study, cetrimonium chloride (CAS No. 112-02-7) was dermally applied to mated female New Zealand White rabbits from GD 7–18 at dose levels of 0, 10, 20 and 40 mg/kg bw/day for two hours/day. Following application, the application site was rinsed with water and dried. Apart from skin effects at the application site, no maternal or foetal signs of toxicity were observed during the study. Skin irritation at the application site was noted at all doses with dose-related severity and duration including erythema, oedema, desquamation, atonia, and coriaceousness. The NOAEL for maternal systemic toxicity as well as for developmental toxicity was established as 40 mg/kg bw/day (no effects at the highest tested dose) (SCCS, 2009).

In another developmental toxicity study, stearyl trimethyl ammonium chloride (CAS No. 112-03-8) was dermally applied to mated female SD rats from GD 6–15 at dose levels of 4.5, 7.5 and 12.5 mg/kg bw/day. The chemical was applied with a syringe (gently massaged into the shaved area) and left on the skin. Systemic maternal or foetal signs of toxicity were not noted during the study. Skin irritation was noted at the site of application and was considered to be as a result of local irritation and not indicative of systemic toxicity. The NOAEL for maternal systemic toxicity as well as for developmental toxicity was established as 12.5 mg/kg bw/day (no effects at the highest tested dose) (SCCS, 2009).

# **Risk Characterisation**

#### **Critical Health Effects**

The critical health effects for risk characterisation include systemic acute effects (acute toxicity from oral and dermal exposure) and concentration-dependent local effects (corrosivity).

#### **Public Risk Characterisation**

Although the use of chemicals in this group in cosmetic and domestic products in Australia is not known, chemicals in this group have reported cosmetic and domestic uses overseas (see **Import**, **manufacture and use**). Considering the range of domestic and cosmetic products that may contain these chemicals in Australia, the main route of public exposure is expected to be through the skin and eyes, inhalation from products applied as cosmetics and from using domestic products.

Even though the concentration of the chemicals in this group in cosmetic products is not reported, considering the reported concentration of 2.4 % of C12–16 alkyldimethylbenzylammonium chloride (CAS No. 68424-85-1) in personal care products, the concentrations are not considered to be sufficiently high to cause any significant human health effects. Whilst a much higher concentration of chemicals in this group has been reported for domestic uses (up to 32 %), provided that normal precautions are taken to avoid eye contact and inhaling chemical vapours, the risk from the use of domestic products is not considered to be unreasonable.

Therefore, the risk to public health is not considered to be unreasonable and further risk management is not considered necessary for public safety.

# **Occupational Risk Characterisation**

During product formulation, dermal, ocular and inhalation exposure of workers to the chemical can occur, particularly where manual or open processes are used. These might include transfer and blending activities, quality control analysis, and cleaning and maintaining equipment. Worker exposure to the chemical at lower concentrations could also occur while using formulated products containing the chemical. The level and route of exposure will vary depending on the method of application and work practices employed.

Given the critical health effects, the chemical could pose an unreasonable risk to workers unless adequate control measures to minimise dermal, ocular and inhalation exposure to the chemical are implemented. The chemical should be appropriately classified and labelled to ensure that a person conducting a business or undertaking (PCBU) at a workplace (such as an employer) has adequate information to determine appropriate controls.

The data available support an amendment to the hazard classification in HSIS (see **Regulatory control: occupational health and safety**) (refer to the **Recommendation** section).

# **NICNAS** Recommendation

Assessment of the chemicals in this group is considered to be sufficient, provided that the recommended amendment to the classification is adopted, and labelling and all other requirements are met under workplace health and safety and poisons legislation as adopted by the relevant state or territory.

# **Regulatory Control**

Work Health and Safety

The chemicals are recommended for classification and labelling under the current approved criteria and adopted GHS as below. This assessment does not consider classification of physical hazards and environmental hazards. This is the existing classification for CAS No. 63449-41-2.

#### Note:

Whilst the acute oral toxicity (R22) and corrosivity (R34) classification is the existing classification for didecyl dimethyl ammonium chloride (CAS No: 7173-51-5) and alkyl dimethyl benzyl ammonium chloride (CAS No: 63449-41-2), this should be applied to all members of this group.

Similarly, whilst the acute dermal toxicity (R21) classification is the existing classification for alkyl dimethyl benzyl ammonium chloride (CAS No: 63449-41-2), this should also be applied to all members of this group.

Hazard	Approved Criteria (HSIS) <sup>a</sup>	GHS Classification (HCIS) <sup>b</sup>
Acute Toxicity	Harmful if swallowed (Xn; R22) Harmful in contact with skin (Xn; R21)	Harmful if swallowed - Cat. 4 (H302) Harmful in contact with skin - Cat. 4 (H312)
Irritation / Corrosivity	Causes burns (C; R34)	Causes severe skin burns and eye damage - Cat. 1B (H314)

<sup>&</sup>lt;sup>a</sup> Approved Criteria for Classifying Hazardous Substances [NOHSC:1008(2004)].

#### Advice for consumers

Products containing chemicals in this group should be used according to the instruction on the label.

# Advice for industry

# Control measures

Control measures to minimise the risk from dermal, ocular, and inhalation exposure to the chemicals should be implemented in accordance with the hierarchy of controls. Approaches to minimise risk include substitution, isolation and engineering controls. Measures required to eliminate or minimise risk arising from storing, handling and using a hazardous chemical depend on the physical form and the manner in which the chemical is used. Examples of control measures which may minimise the risk include, but are not limited to:

- using closed systems or isolating operations;
- using local exhaust ventilation to prevent the chemicals from entering the breathing zone of any worker;
- minimising manual processes and work tasks through automating processes;
- work procedures that minimise splashes and spills;
- regularly cleaning equipment and work areas; and
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemical.

Guidance on managing risks from hazardous chemicals are provided in the *Managing risks of hazardous chemicals in the workplace—Code of practice* available on the Safe Work Australia website.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

<sup>&</sup>lt;sup>b</sup> Globally Harmonized System of Classification and Labelling of Chemicals (GHS) United Nations, 2009. Third Edition.

<sup>\*</sup> Existing Hazard Classification. No change recommended to this classification

#### Obligations under workplace health and safety legislation

Information in this report should be taken into account to assist with meeting obligations under workplace health and safety legislation as adopted by the relevant state or territory. This includes, but is not limited to:

- ensuring that hazardous chemicals are correctly classified and labelled;
- ensuring that (material) safety data sheets ((m)SDS) containing accurate information about the hazards (relating to both health hazards and physicochemical (physical) hazards) of the chemical are prepared; and
- managing risks arising from storing, handling and using a hazardous chemical.

Your work health and safety regulator should be contacted for information on the work health and safety laws in your jurisdiction.

Information on how to prepare an (m)SDS and how to label containers of hazardous chemicals are provided in relevant codes of practice such as the *Preparation of safety data sheets for hazardous chemicals*— *Code of practice* and *Labelling of workplace hazardous chemicals*—*Code of practice*, respectively. These codes of practice are available from the Safe Work Australia website.

A review of the physical hazards of the chemicals has not been undertaken as part of this assessment.

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Last Update 03 July 2015

# **Chemical Identities**

Chemical Name in the Inventory and Synonyms	1-Hexadecanaminium, N,N,N-trimethyl-, bromide cetrimonium bromide cetyl trimethyl ammonium bromide hexadecyltrimethylammonium bromide hexadecyl(trimethyl)ammonium bromide ammonium, hexadecyltrimethyl-, bromide	
CAS Number	57-09-0	
Structural Formula		

	H <sub>1</sub> C CH <sub>1</sub>
Molecular Formula	C19H42N.Br
Molecular Weight	364.45

Chemical Name in the Inventory and Synonyms	1-Dodecanaminium, N,N,N-trimethyl-, chloride trimethyldodecylammonium chloride dodecyltrimethylammonium chloride lauryl trimethyl ammonium chloride ammonium, dodecyltrimethyl-, chloride
CAS Number	112-00-5
Structural Formula	

	H <sub>3</sub> C CH <sub>3</sub>
Molecular Formula	C15H34N.CI
Molecular Weight	263.89

Chemical Name in the Inventory and Synonyms	1-Hexadecanaminium, N,N,N-trimethyl-, chloride cetrimonium chloride cetyl trimethyl ammonium chloride trimethylhexadecylammonium chloride
CAS Number	112-02-7
Structural Formula	

J4/2020	H <sub>1</sub> C
Molecular Formula	C19H42N.CI
Molecular Weight	320

Chemical Name in the Inventory and Synonyms	1-Octadecanaminium, N,N,N-trimethyl-, chloride quaternium-10 trimethyloctadecylammonium chloride stearyl trimethyl ammonium chloride steartrimonium chloride
CAS Number	112-03-8
Structural Formula	

J-1/2020	IWAI Group Assessment Report
Molecular Formula	C21H46N.CI
Molecular Weight	348.05

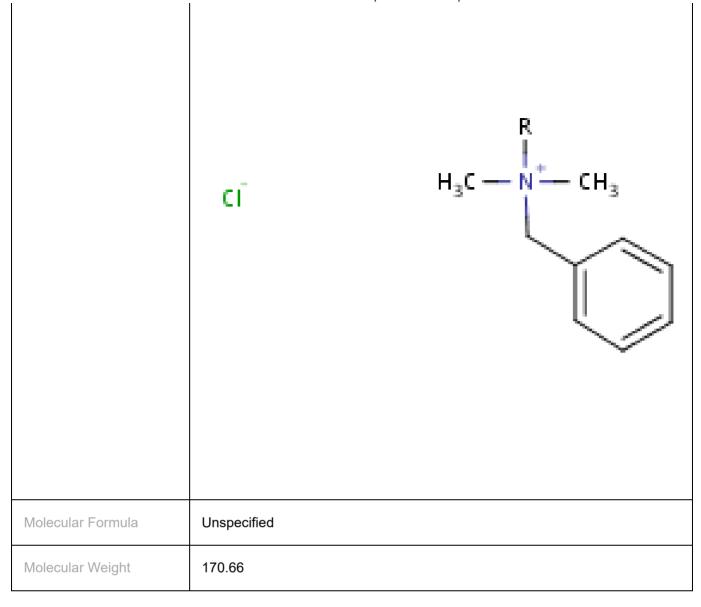
Chemical Name in the Inventory and Synonyms	1-Dodecanaminium, N,N,N-trimethyl-, bromide laurtrimonium bromide dodecyltrimethylammonium bromide ammonium, dodecyltrimethyl-, bromide
CAS Number	1119-94-4
Structural Formula	

14/2020	H <sub>3</sub> C  H <sub>3</sub> C  CH <sub>3</sub>
Molecular Formula	C15H34N.Br
Molecular Weight	308.35

Chemical Name in the Inventory and Synonyms	1-Decanaminium, N-decyl-N,N-dimethyl-, chloride didecyl dimethyl ammonium chloride ammonium, didecyldimethyl-, chloride didecyldimethyl-ammonium chloride
CAS Number	7173-51-5
Structural Formula	

14/2020	H.E. CH. CH.
Molecular Formula	C22H48N.CI
Molecular Weight	362.08

Chemical Name in the Inventory and Synonyms	Quaternary ammonium compounds, alkylbenzyldimethyl, chlorides benzalkonium chloride ammonium, alkyldimethylbenzyl-, chloride mixture of alkylbenzyldimethylammonium compounds
CAS Number	8001-54-5
Structural Formula	



Chemical Name in the Inventory and Synonyms	1-Docosanaminium, N,N,N-trimethyl-, chloride behentrimonium chloride docosyltrimethylammonium chloride ammonium, docosyltrimethyl-, chloride behenyltrimethylammonium chloride
CAS Number	17301-53-0
Structural Formula	

	H <sub>I</sub> C=N=CH <sub>i</sub>
Molecular Formula	C25H54N.CI
Molecular Weight	404.16

Chemical Name in the Inventory and Synonyms	Quaternary ammonium compounds, benzylcoco alkyldimethyl, chlorides alkyl dimethyl benzyl ammonium chloride benzyl chloride quaternary salt of N,N-dimethylcocoamine dimethyl cocobenzyl ammonium chloride dimethylcocobenzalkonium chloride coco alkyldimethylbenzyl ammonium chlorides
CAS Number	61789-71-7
Structural Formula	No Structural Diagram Available

Molecular Formula	Unspecified
Molecular Weight	

Chemical Name in the Inventory and Synonyms	Quaternary ammonium compounds, benzyl-C8-18-alkyldimethyl, chlorides C8-18-alkydimethylbenzyl ammonium chlorides alkyl dimethyl benzyl ammonium chloride benzyldimethyl(mixed alkyl)ammonium chloride benzyl-C8-18-alkyldimethylammonium chloride
CAS Number	63449-41-2
Structural Formula	No Structural Diagram Available
Molecular Formula	Unspecified
Molecular Weight	

Chemical Name in the Inventory and Synonyms	Quaternary ammonium compounds, benzyl-C12-18-alkyldimethyl,chlorides C12-18 alkyl dimethyl benzyl ammonium chloride alkyl (C12-18) dimethylbenzyl ammonium chloride benzyl-C12-18-alkyldimethyl ammonium chloride
CAS Number	68391-01-5
Structural Formula	

Molecular Formula

Molecular Weight

# No Structural Diagram Available Unspecified 377.80

Chemical Name in the Inventory and Synonyms	Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl,chlorides C12-16 alkyldimethylbenzylammonium chloride benzyl-C12-16-alkyl dimethyl ammonium chlorides alkyl (C12-16) dimethylbenzyl ammonium chloride dimethylbenzyl-ammonium chloride
CAS Number	68424-85-1
Structural Formula	No Structural Diagram Available
Molecular Formula	Unspecified
Molecular Weight	359.60

Chemical Name in the Inventory and Synonyms

Quaternary ammonium compounds, benzyl-C12-18-alkyldimethyl,salts with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1) (C12-18) alkyldimethylbenzylammonium saccharinate Quaternium-3

04/2020	IMAP Group Assessment Report myristalkonium saccharinate
CAS Number	68989-01-5
Structural Formula	
Molecular Formula	C7H5NO3S.
Molecular Weight	514.77

Chemical Name in the Inventory and Synonyms	Quaternary ammonium compounds, benzyl-C12-14-alkyldimethyl,chlorides alkylbenzyldimethylammonium chlorides, benzyl-C12-14-alkyldimethy benzyl-C12-14-alkyldimethylammonium chlorides barquat OJ
CAS Number	85409-22-9
Structural Formula	

# No Structural Diagram Available Molecular Formula Unspecified Molecular Weight

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