

Lead(2+) salts of medium-chain carboxylic acids: Environment tier II assessment

27 November 2014

CAS Registry Numbers: 15696-43-2, 64504-12-7, 27253-41-4, 20403-42-3, 27253-28-7, 15306-30-6, 16996-40-0.



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Preface

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

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

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

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

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

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

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

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

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

Disclaimer

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Acronyms & Abbreviations

Grouping Rationale

This Tier II assessment considers the environmental risks associated with the industrial uses of the lead salts of seven closely related carboxylic acids:

Octanoic acid, lead salt (Lead octanoate)
Isooctanoic acid, lead salt (Lead isooctanoate)
Isononanoic acid, lead salt (Lead isononanoate)
Decanoic acid, lead salt (Lead decanoate)
Neodecanoic acid, lead salt (Lead neodecanoate)
Dodecanoic acid, lead salt (Lead laurate)
Hexanoic acid, 2-ethyl-, lead salt (Lead octoate)

The chemicals in this group are related to the chemicals assessed as part of the 1:2 Lead(2+) Salts of Medium-Chain Carboxylic Acids group. Both groups of chemicals are structurally similar, but they may have some minor compositional differences. Although they have been assessed as separate groups, persons interested in the chemicals assessed here should also consider those assessed under the 1:2 Lead(2+) Salts of Medium-Chain Carboxylic Acids group assessment. The chemicals previously assessed under the defined stoichiometry group are used as analogue chemicals throughout this assessment.

The parent carboxylic acids for these salts are medium-chain (C₆₋₁₂) naturally occurring straight-chain fatty acids and synthetically produced fatty acids with branched chains. The lead salts of these acids are a subset of a large class of industrially important metal salts of fatty acids collectively identified as metal soaps. This subset of metal soaps is of indefinite chemical

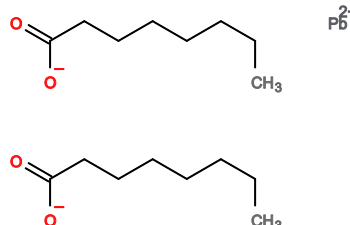
composition based on their Chemical Abstracts Service chemical names and formulae as listed in the Australian Inventory of Chemical Substances (the Inventory), and they can contain free fatty acids and/or other counterions in addition to the stoichiometric lead salts.

The risk assessment of these chemicals has been conducted as a group because all seven substances are lead (predominantly in the 2+ oxidation state) salts of structurally and chemically similar medium-chain fatty acids. Although these salts are sparingly soluble in water, they can all potentially release lead(2+) ions which provides a common source of toxicity for each of these substances. Furthermore, the potential environmental exposure pathways for chemicals in this group are similar based on specific industrial uses as driers in coating products such as paints, lacquers and varnishes. Based on these considerations, the chemicals in this group are each expected to have generally similar environmental fate and ecotoxicity profiles.

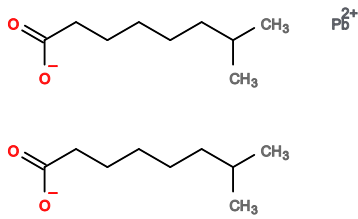
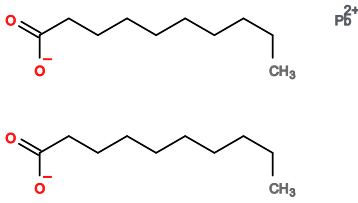
Chemical Identity

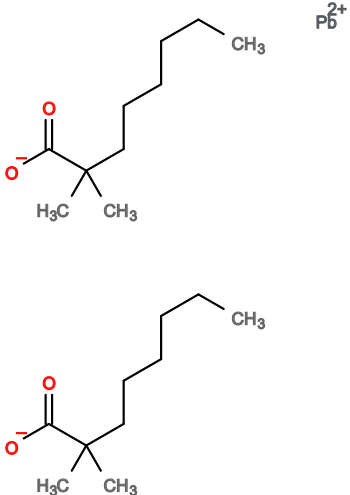
Based on available chemical composition data for this group of lead salts (Nora and Koenen, 2012), each salt is composed of lead(2+) ions and carboxylic acid anions in a ratio of approximately 1:2. The chemical identity information provided below for each salt therefore assumes an idealised 1:2 ratio of lead(2+) cations to the respective carboxylate mono-anions. However, it is noted that the chemical composition of lead fatty acid soaps in this group, such as the quantities of free fatty acid present, may vary depending on the manufacturing method employed and the specific requirements of the end-use application.

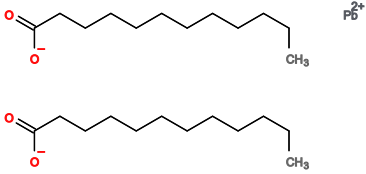
Neodecanoic acid (CAS RN 26896-20-8) is a mixture of branched isomers which contain a quaternary carbon. The mixture of isomers of neodecanoic acid made industrially may be categorised as trialkylacetic acids with the general formula $R_1R_2R_3CCOOH$. The same representative structure for neodecanoic acid identified in the United States Environmental Protection Agency assessment of neoacids C5–C28 category undertaken for the High Production Volume (HPV) chemicals programme has been selected for the assessment of the organic components of the lead salt of neodecanoic acid (US EPA, 2009). However, it is noted that lead salts of neodecanoic acid will contain other highly branched isomers of decanoic acid than the one depicted. Similarly, representative structures are given for the isooctanoate and isononanoate anions.

CAS RN	15696-43-2
Chemical Name	Octanoic acid, lead salt
Synonyms	Lead octanoate Lead caprylate
Representative Structural Formula	
Representative Molecular Formula	$C_{16}H_{30}O_4Pb$

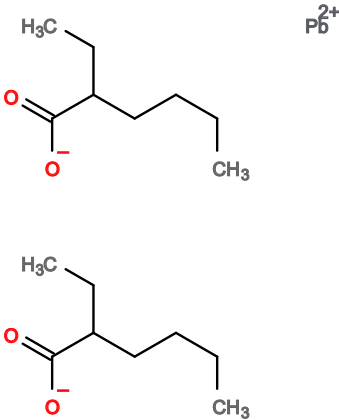
Representative Molecular Weight (g/mol)	493.61
Representative SMILES	[Pb ⁺⁺].CCCCCCCC(=O)[O-].CCCCCCCC(=O)[O-]
CAS RN	64504-12-7
Chemical Name	Isooctanoic acid, lead salt
Synonyms	Lead isooctanoate
Representative Structural Formula	<p>The structural formula shows a central lead ion (Pb²⁺) coordinated to two isooctanoate anions. Each isooctanoate anion is represented as a carboxylate group (COO⁻) attached to a seven-carbon chain with two methyl groups at the 3-position (isooctanoate).</p>
Representative Molecular Formula	C ₁₆ H ₃₀ O ₄ Pb
Representative Molecular Weight (g/mol)	493.61
Representative SMILES	[Pb ⁺⁺].CC(C)CCCCC(=O)[O-].CC(C)CCCCC(=O)[O-]
CAS RN	27253-41-4
Chemical Name	Isononanoic acid, lead salt

Synonyms	Lead isononanoate
Representative Structural Formula	
Representative Molecular Formula	C ₁₈ H ₃₄ O ₄ Pb
Representative Molecular Weight (g/mol)	521.66
Representative SMILES	[Pb++].CC(C)CCCCC(=O)[O-].CC(C)CCCCC(=O)[O-]
CAS RN	20403-42-3
Chemical Name	Decanoic acid, lead salt
Synonyms	Lead decanoate Lead caprate
Representative Structural Formula	
Representative Molecular Formula	C ₂₀ H ₃₈ O ₄ Pb

Representative Molecular Weight (g/mol)	549.71
Representative SMILES	[Pb ⁺⁺].CCCCCCCCC(=O)[O-].CCCCCCCCC(=O)[O-]
CAS RN	27253-28-7
Chemical Name	Neodecanoic acid, lead salt
Synonyms	Lead neodecanoate
Representative Structural Formula	
Representative Molecular Formula	C ₂₀ H ₃₈ O ₄ Pb
Representative Molecular Weight (g/mol)	549.71
Representative SMILES	[Pb ⁺⁺].CCCCCCC(C)(C)C(=O)[O-].CCCCCCC(C)(C)C(=O)[O-]

CAS RN	15306-30-6
Chemical Name	Dodecanoic acid, lead salt
Synonyms	Lead laurate Lead dodecanoate
Representative Structural Formula	
Representative Molecular Formula	C ₂₄ H ₄₆ O ₄ Pb
Representative Molecular Weight (g/mol)	605.82
Representative SMILES	[Pb++].CCCCCCCCCCCC(=O)[O-]. CCCCCCCCCCCC(=O)[O-]

CAS RN	16996-40-0
Chemical Name	Hexanoic acid, 2-ethyl-, lead salt
Synonyms	Lead octoate Lead 2-ethylhexanoate
Representative Structural Formula	

	
Representative Molecular Formula	C ₁₆ H ₃₀ O ₄ Pb
Representative Molecular Weight (g/mol)	493.61
Representative SMILES	[Pb++].CCCCC(CC)C(=O)[O-].CCCCC(CC)C(=O)[O-]

Physical and Chemical Properties

There is only limited information available on the physical properties of the chemicals addressed in this group assessment. Available industry sources suggest lead octoate is sold commercially in a series of lead concentrations, commonly ranging from 24% w/w to 36% w/w total lead. All variants are described as liquids under ambient conditions. The pure 1:2 lead(2+) salts of the majority of the fatty acids in this group are expected to be solids under ambient conditions based on the typical properties of metal soaps (Nora and Koenen, 2012). Data available for the analogous 1:2 lead(2+) salts of the fatty acids in this group have been used to characterise the physical and chemical properties of the chemical considered here.

The metal soaps of divalent (2+) metal ions are well known to be only sparingly soluble in water (Nora and Koenen, 2012). A number of studies of the solubility of various divalent metal soaps show the lead(2+) soaps typically dissociate in water to form lead(2+) ions and fatty acids in the form of carboxylate mono-anions. These studies also clearly demonstrate that the water solubility of metal soaps decreases as the length of the fatty acid carbon chain increases. Additionally, these studies have shown that the lead(2+) salts are typically the least soluble of the divalent metal salts of fatty acids (Hunter and Liss, 1976; Mauchauffee, et al., 2008).

No quantitative water solubility data have been identified for the chemicals in this group. However solubility products (K_{sp} s), which are a quantitative measure of the position of the solubility equilibrium, are available for lead dioctanoate (CAS RN 7319-86-0), lead didecanoate (CAS RN 15773-52-1) and lead dilaurate (CAS RN 15773-55-4) (Hunter and Liss, 1976; Mauchauffee, et al., 2008). All measurements were obtained at an ionic strength of 0.1 M (NaCl). The values for lead dioctanoate and lead didecanoate (a) were obtained at 20°C, while those for lead didecanoate (b) and lead dilaurate were obtained at 25°C. The concentrations of lead(2+) ions at saturation (at 20°C) for lead dioctanoate and lead didecanoate (a) were reported by the authors (Mauchauffee, et al., 2008). The lead(2+) ion concentration at saturated (at 25°C) for lead didecanoate (b) and lead dilaurate were calculated using an activity coefficient of 0.586 M, as used in the original study (Hunter and Liss, 1976):

Chemical	Lead dioctanoate	Lead didecanoate	Lead dilaurate
K_{sp}	1.58×10^{-11}	(a) 8.51×10^{-17} (b) 3.16×10^{-13}	5.01×10^{-16}
Lead(2+) Concentration at Saturation	36.05 mg/L	(a) 1.34 mg/L (b) 15.18 mg/L	1.77 mg/L

These values are considered to represent the solubility of any 1:2 lead(2+) salts of octanoic acid, decanoic acid and lauric acid contained in lead octanoate, lead decanoate and lead laurate, respectively. Based on the observed trend in solubility for metal soaps, any 1:2 lead(2+) salts of the branched fatty acids (C₈₋₁₀) in this group are expected to have solubility equal to or greater than that of the 1:2 lead(2+) salt of lauric acid (C₁₂). The presence of impurities in the chemicals in this group may influence their overall solubilities. However, these data are expected to be generally representative of the availability of lead(2+) in water for the lead salts in this group.

Import, Manufacture and Use

Australia

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

International

Lead octoate, lead isooctanoate, lead neodecanoate and lead octanoate have been reported to be used internationally in paints and surface coatings. Lead octoate appears to be primarily used in the fabricated metal products sectors, with lead octanoate reported to be used in the construction industry. Lead isooctanoate has been reported to be used in the electricity, gas, steam and air conditioning sector, with some use also reported in anti-fouling paint for ships (Nordic Council of Ministers, 2013).

Lead octoate, lead isooctanoate and lead octanoate were reported to be used in Denmark, Norway and/or Sweden in 2011. Each chemical was reported to be used at a volume of 0.1 tonnes or less. Lead neodecanoate was reported to be used in Norway between 2001 and 2009 at a similar volume, but use has not been reported in more recent years. Similarly, lead isononanoate was reported to be used in Sweden between 1993 and 2003, but recent use has not been reported. The use pattern for this chemical was not specified (Nordic Council of Ministers, 2013).

No use data were available for lead decanoate and lead laurate. These chemicals do not appear to be used industrially in Canada and have not been introduced for an industrial use at a volume greater than 100 kg per annum in Sweden since its records began in 1992 (Environment Canada, 2013a; Keml, 2014). Further, all chemicals in this group are currently only pre-registered under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation. Therefore, it can be assumed that these chemicals are not currently being used at a volume greater than 100 tonnes per annum in the European Union (ECHA, 2014c; 2014d).

Environmental Regulatory Status

Australia

Lead and lead compounds are subject to reporting under the Australian National Pollutant Inventory (NPI). Under the NPI, emissions of lead and lead compounds are required to be reported annually by facilities that use or emit more than 10 tonnes of lead or lead compounds, burn more than 2000 tonnes of fuel, consume more than 60 000 megawatt hours of electricity (excluding lighting and motive purposes), or have an electricity rating of 20 megawatts during a reporting year (Australian Government Department of the Environment, 2013a). Emissions may be intentional, accidental or incidental releases arising through industrial processes. Additionally, emissions of lead and lead compounds from diffuse sources, such as lawn mowers and wood heaters, are also periodically estimated by state environment authorities. Diffuse emissions data are updated much less frequently than facility data (Australian Government Department of the Environment, 2013b).

The *Uniform Paint Standard* of the *Poisons Standard 2013* (Cwlth) restricts lead and lead compounds to a maximum of 0.1% of the non-volatile content of all paints manufactured and sold in Australia (measured as elemental lead) (Commonwealth of Australia, 2013).

United Nations

None of the chemicals in this group are currently identified as a Persistent Organic Pollutant (UNEP, 2001), ozone depleting substance (UNEP, 1985), or hazardous substance for the purpose of international trade (UNEP & FAO, 1998).

The United Nations Environment Programme (UNEP), in partnership with the World Health Organization (WHO), has established the Global Alliance to Eliminate Lead Paint. The alliance primarily supports actions in developing nations to reduce and phase-out lead use in paints (UNEP, 2011).

OECD

None of the chemicals in this group have been sponsored for assessment under the Cooperative Chemicals Assessment Programme (CoCAP) (OECD, 2013).

Canada

Lead octoate and lead neodecanoate were categorised as Persistent (P), not Bioaccumulative (not B), and Inherently Toxic to the Environment (iT_E) by Environment Canada during the Categorization of the Domestic Substances List (DSL) (Environment Canada, 2013b). A subsequent screening assessment is yet to be completed (Environment Canada, 2013c).

The remaining chemicals in this group are not currently listed on the DSL (Environment Canada, 2013a).

Lead in most paint products available to consumers in Canada is limited to 90 mg/kg (0.009% w/w) of the non-volatile content under the *Surface Coating Materials Regulations* of the *Canada Consumer Product Safety Act 2010*. Exempted products which contain more than 90 mg/kg lead must be appropriately labelled (Government of Canada, 2005).

European Union

All chemicals in this group have been pre-registered, but not yet undergone the full registration process, under the REACH legislation (ECHA, 2014g). None of the chemicals in this group are currently identified as a Substance of Very High Concern in the European Union.

However, it is noted that all other lead compounds currently registered under the REACH legislation (for example, mixed C₁₆₋₁₈ lead carboxylates (CAS RN 91031-62-8)) have been identified as Substances of Very High Concern due to their reproductive toxicity, and are currently included on the Candidate List for Eventual Inclusion in Annex XIV (the Authorisation List) to REACH (ECHA, 2013).

United States of America

Select industries in the United States of America (USA), including most mining, utilities and manufacturing facilities, must report emissions of lead and lead compounds to the United States Environmental Protection Agency (US EPA) if the facility manufactures or processes more than 25 000 pounds of lead compounds (approximately 11 tonnes) per annum. Reporting is also required if the facility otherwise uses more than 10 000 pounds (approximately 4.5 tonnes) in a reporting year (US EPA, 2012; 2014a; 2014b).

Most paint products containing lead, as well as toys and furniture painted using such products, are prohibited in the USA if the lead content exceeds 0.009% w/w of the non-volatile paint content under the *Consumer Product Safety Improvement Act 2008*. Exempted products which contain more than 0.009% w/w lead must be appropriately labelled (United States Government, 2008).

Environmental Exposure

Based on the available data, the principal industrial uses of lead octoate, lead isooctanoate, lead neodecanoate and lead octanoate are in industrial coatings, such as paints, lacquers and varnishes. Metal soaps are known to be used as driers in coatings containing drying oil components, with lead soaps typically used at a concentration of 0.5% w/w lead (non-volatile content) (Australian Government Department of the Environment, 2014; Bielman, 1993). However, the use of these chemicals in industrial coatings in Australia at concentrations resulting in greater than 0.1% w/w lead (non-volatile content) is not allowed under the *Uniform Paints Standard* (Commonwealth of Australia, 2013). Therefore, current industrial use of these chemicals as driers in surface coatings in Australia does not occur.

The extent of use of the remaining chemicals in this group in Australia is unclear. Based on the use information available for the above chemicals, international data and the chemical similarity of the substances addressed in this group assessment, the remaining chemicals are assumed to also primarily be used in industrial coating products. However, the restrictions on lead compounds in paints under the *Uniform Paint Standard*, and an increased awareness of the environmental and human health concerns of lead pollution, will preclude current uses of these chemicals in industrial coating products in Australia.

When present in existing industrial coatings, the primary source of environmental exposure for the chemicals in this group is expected to be release of soluble lead(2+) ions from the cured coating. A range of studies have highlighted the potential for lead to be released from intact coatings (Barnes and Davis, 1996; Beauchemin, et al., 2011; Davis and Burns, 1999). Chips and dust from coatings containing lead can also result in environmental exposure of lead compounds. A small proportion may also be released to sewer, surface water or soil during application and disposal of excess product (OECD, 2009).

Environmental Fate

Dissolution, Speciation and Partitioning

The behaviour of the lead(2+) ion is strongly dependent on the chemistry of the environmental compartment into which it is released.

The metal soaps are salts of weak acids and dissolution of these substances in water therefore results in hydrolysis. Hydrolysis of the fatty acid conjugate base results in the formation of the corresponding fatty acid. The extent to which this reaction occurs is dependent on the properties of the acid and the pH of the aquatic environment. At neutral pH, fatty acids are predominantly in the conjugate base (anionic) form. Any free fatty acids present in these chemicals will similarly exist as the conjugate base at neutral pH. For the metal ion, hydrolysis is a result of dissociation of hydrogen ions from water molecules coordinated to the metal ion. In the case of lead(2+) ions, coordinated water is only weakly acidic and the predominant form of the dissolved metal ion in pure water at neutral pH is the simple hydrated lead(2+) di-cation (Mauchauffee, et al., 2008).

However, in environmental waters, lead(2+) ions are expected to undergo a range of additional reactions and they can therefore exist as a variety of different chemical species. The speciation chemistry of lead(2+) ions in environmental waters is complex and strongly dependent on water chemistry, especially pH and the presence of complexing anions. For example, at pH levels lower than 7, the simple hydrated lead(2+) di-cation is the dominant species of ionic lead (ANZECC, 2000a). However, at pH levels greater than 7, the speciation of ionic lead is dominated by the formation of carbonate complexes, such as PbCO_3 (US EPA, 1999). These carbonate complexes have low solubility and the precipitation of lead(2+) salts becomes important under

alkaline conditions. In seawater, lead(2+) is complexed by chloride ions. These complexes account for more than 90% of the speciation of ionic lead in seawater (ANZECC, 2000a).

In addition to complexation by simple inorganic anions, lead(2+) is complexed by organic matter in environmental waters. These complexes are of great significance for the environmental fate of lead(2+) because they account for the majority of dissolved lead in natural freshwater at pH values in the range 5 to 9 (ANZECC, 2000a). Further, the partitioning of lead(2+) from the water phase onto clay particles, particulate humic substances, and iron, aluminium and manganese (oxy)hydroxides have all been identified as important mechanisms controlling the concentration of lead in natural waters. In sediments, the speciation of lead will be dominated by complexation by humic substances and the formation of relatively insoluble lead sulfides (ANZECC, 2000a).

The partitioning behaviour of lead in soil has a complex dependence on soil properties, but is mainly determined by pH and clay content. A detailed review of measured partition coefficients for sorption from water onto soil (K_{Ds}) conducted by the US EPA identified values for lead(2+) in the range of 150 L/kg to 44 580 L/kg. The adsorption of lead on soil generally increases with increasing soil pH (US EPA, 1999). Lead is typically considered relatively immobile in soil (UNEP, 2010).

Biotransformation

The straight-chain and branched-chain organic components of the salts in this group are expected to be biodegradable both as the lead salts and as the free fatty acids.

No biodegradation data were available for any chemicals in this group. However, a ready biodegradation study on the analogue chemical lead bis(2-ethylhexanoate) (CAS RN 301-08-6), conducted in accordance with OECD Test Guideline (TG) 301C, found the chemical to undergo 98% degradation in 28 days (LMC, 2013; NITE, 2014).

The straight-chain and iso-branched fatty acid components of the chemicals in this group will undergo relatively rapid biodegradation in the environment. Available experimental data from studies conducted in accordance with standard test guidelines demonstrate that dodecanoic acid (lauric acid), 2-ethylhexanoic acid and octanoic acid are all readily biodegradable (63-73% degradation in 15 days, OECD TG 301D; 99% degradation in 28 days, OECD TG 301E and >60% degradation in 10 days, OECD TG 301D, respectively) (ECHA, 2014b; 2014e; 2014f). The available biodegradation data for short-chain isocarboxylic acids suggest that the biodegradation potential of the remaining isocarboxylic acids in this group should not be expected to differ significantly from that of their straight-chain analogues (LMC, 2013).

Neodecanoic acid is not expected to be readily biodegradable, with a study conducted in accordance with OECD TG 301F finding the chemical to undergo 11% degradation in 28 days (US EPA, 2006). Additional studies have provided similar results (ECHA, 2014h). This is to be expected, as the highly branched structure of this chemical likely inhibits microbial oxidation.

Bioaccumulation

Chemicals in this group will release lead ions, which bioaccumulate in most organisms.

The lead(2+) ions released from these chemicals may pose a bioaccumulation hazard depending on the bioavailability of the metal ion under the prevailing exposure conditions. Conventional measures of bioaccumulation as applied to organic chemicals are not appropriate for metal ions. These measures do not consider the potential for metals to accumulate in specific tissues, the physiological mechanisms available to organisms to regulate internal metal concentrations, and the influence of environmental factors (US EPA, 2007). Nevertheless, lead and lead compounds are globally acknowledged to pose a significant bioaccumulation concern (UNEP, 2010; 2014).

The fatty acid components of the chemicals in this group are not expected to pose a bioaccumulation hazard. The straight-chain fatty acids of the chemicals in this group are dietary fatty acids which are naturally ubiquitous in the environment and organisms, and their storage in body tissues is an essential biological process which is regulated by homeostatic controls (NRC, 2005). The extent to which the branched fatty acids are similarly metabolised and stored in organisms is unclear. However, the structural properties and degradability of most of these chemicals suggest limited potential for bioaccumulation. The chemical characteristics of these fatty acids are similar to those of anionic surfactants, which are generally considered not to be bioaccumulative (Konnecker, et al., 2011). This is supported by a measured bioconcentration factor (BCF) of less than 225 for neodecanoic acid in the fish *Oncorhynchus mykiss* (ECHA, 2014h).

Transport

The chemicals in this group and their ionic components have a low potential for long-range transport.

The lead salts of fatty acids are ionic solids that do not partition to the atmospheric compartment, where long-range transport typically occurs. The fatty acids constituents of these salts are generally rapidly biodegradable and therefore not subject to long-range transport. The ionic lead components of the salts may have some limited mobility in water due to complexation by dissolved organic matter, but lead released into water and onto soil will eventually become bound to sediment or soil particles (UNEP, 2010).

Predicted Environmental Concentration (PEC)

A PEC was not calculated for the chemicals or their ionic components addressed under this assessment.

Historically, lead compounds in paint have been a significant source of lead in the environment. Further, surfaces previously coated with preparations containing high concentrations of lead compounds continue to release lead to the environment (Davis and Burns, 1999; UNEP, 2011). However, the release of lead compounds from current industrial use of the chemicals in this group is not expected due to restrictions on lead compounds in coating products used in Australia.

The most significant source of potential environmental emissions of lead compounds from paint is expected to be associated with the release of lead during the lifetime, and end-of-life disposal, of coated articles. Studies which have considered the release of lead from outdoor surfaces have found water runoff from surfaces painted between 1994 and 1999 to contain an average of 8.4 micrograms per litre ($\mu\text{g/L}$) of lead (Davis and Burns, 1999). While some runoff water may pass into sewers, a proportion can be expected to be released directly to surface waters or soil. At the end of their useful life, coated articles are expected to be disposed to landfill. This should not be expected to result in significant environmental exposure due to the immobility of lead in soil.

Environmental Effects

No ecotoxicity data specific to the chemicals addressed under this assessment are available. However, it is expected that the environmental effects of sparingly soluble lead salts of fatty acids will be determined principally by the release of lead(2+) ions into the environment. Lead is recognised to be a highly toxic environmental contaminant (UNEP, 2010; 2014). The effects assessment of the chemicals in this group has therefore primarily focused on the extensive body of information regarding the ecotoxicity of lead and inorganic lead compounds.

Effects on Aquatic Life

Bioavailable forms of lead(2+) are very toxic to aquatic life in short and long term exposures.

Toxicity of lead(2+)

The speciation of lead(2+) is strongly dependent on water chemistry, which can have a dramatic effect on the bioavailability and therefore toxicity of lead. For example, lead(2+) is more toxic to freshwater species in soft water than hard water. Toxicity is also higher in acidic freshwater when compared to alkaline freshwater. However, toxicity is lower to marine species than for freshwater species (ANZECC, 2000a). These factors and their effects should be noted when evaluating the toxicity of lead(2+) salts.

The following acute median lethal concentrations (LC50s) and median effective concentration (EC50) for model organisms across three trophic levels for the lead cation were reported in the Registration Dossier for lead metal (CAS RN 7439-92-1) under the European Union REACH legislation (ECHA, 2014a). All studies were conducted on freshwater species using soluble salts of lead(2+):

Taxon	Endpoint	Method
Fish	96 h LC50 = 108 µg Pb/L	Experimental <i>Pimephales promelas</i> (Fathead minnow) ASTM Method; Flow through CaCO ₃ = 43.9 mg/L, pH = 7.4
Invertebrates	48 h LC50 = 73.6 µg Pb/L	Experimental <i>Ceriodaphnia dubia</i> (Water flea) US EPA Method; Semi-static CaCO ₃ = 16.4 mg/L, pH = 5.7
Algae	48 h EC50 = 23.1 µg Pb/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201; Static CaCO ₃ = 24 mg/L, pH = 7.3 Reduced growth rate observed

The chronic toxicity of lead(2+) to freshwater and marine species was critically evaluated for the compilation of water quality trigger values for environmental contaminants in the Australian and New Zealand Guidelines for Fresh and Marine Water Quality. Only studies that considered the complex relationship between water chemistry and toxicity were considered, and no-observed effect concentration (NOEC) equivalent values were derived (ANZECC, 2000a). The equivalent NOEC values available for sensitive freshwater fish and invertebrate species are reported below, along with an effective concentration for 10% of the test population (EC10) value for algae as reported in the Registration Dossier for lead under the European Union REACH legislation (ANZECC, 2000a; ECHA, 2014a):

Taxon	Endpoint	Method
Fish	NOEC = 5.65 µg Pb/L	Experimental <i>Lepidomeda vittatus</i> (Little Colorado spinedace) CaCO ₃ = 30 mg/L
Invertebrates	NOEC = 19.5 µg Pb/L	Experimental <i>Daphnia magna</i> (Water flea) CaCO ₃ = 30 mg/L

Taxon	Endpoint	Method
Algae	48 h EC10 = 4.5 µg Pb/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201; Static CaCO ₃ = 24 mg/L, pH = 7.3 Reduced growth rate observed

Toxicity of medium-chain fatty acids

Apart from octanoic acid, the medium-chain fatty acid constituents of these chemical have only low to moderate toxicity to aquatic life in short and long term exposures.

The following acute LC50 value and EC50 values for model freshwater organisms across three trophic levels for (a) 2-ethylhexanoic acid (CAS RN 149-57-5), (b) octanoic acid (CAS RN 124-07-2), (c) lauric acid (CAS RN 143-07-7) and (d) decanoic acid (CAS RN 334-48-5) were reported in the databases included in the OECD QSAR Toolbox and the Robust Test Summaries submitted to the US EPA under the High Production Volume Challenge Program (LMC, 2013; US EPA, 2001). Additional available toxicity values similarly reflect low to moderate ecotoxicity for these medium-chain fatty acids (LMC, 2013; NITE, 2014):

Taxon	Endpoint	Method
Fish	(a) 96 h LC50 = 70 mg/L	Experimental <i>Pimephales promelas</i> (Fathead minnow) APHA Method 231; Static
	(b) 96 h LC50 = 22 mg/L	Experimental <i>Lepomis macrochirus</i> (Bluegill) US EPA Method; Static
	(c) 96 h LC50 = 5 mg/L	Experimental <i>Oryzias latipes</i> (Japanese medaka) OECD TG 203

Taxon	Endpoint	Method
Invertebrates	(a) 48 h LC50 = 85.4 mg/L	Experimental <i>Daphnia magna</i> (Water flea) EU Method; Static
	(b) 48 h EC50 = 550 mg/L (c) 48 h EC50 = 3.6 mg/L	Experimental <i>Daphnia magna</i> (Water flea) OECD TG 202 Decreased mobility observed
Algae	(a) 72 h EC50 = 49.3 mg/L	Experimental <i>Desmodesmus subspicatus</i> (Green algae) DIN 38412 L9; Static Reduced growth rate observed
	(b) 72 h EC50 = 31 mg/L (d) 72 h EC50 = 5.9 mg/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201 Reduced growth rate observed

The following chronic NOEC and EC10 values for model organisms across two trophic levels for (a) 2-ethylhexanoic acid, (b) octanoic acid, (c) lauric acid and (d) decanoic acid were reported in the databases included in the OECD QSAR Toolbox and the Robust Test Summaries submitted to the US EPA under the High Production Volume Challenge Program (LMC, 2013; US EPA, 2001):

Taxon	Endpoint	Method
Invertebrates	(a) 21 d NOEC = 25 mg/L (c) 21 d NOEC = 0.47 mg/L (d) 21 d NOEC = 0.20 mg/L	Experimental <i>Daphnia magna</i> (Water flea) OECD TG 211 Reproductive toxicity observed

Taxon	Endpoint	Method
Algae	(a) 72 h EC10 = 31.9 mg/L	Experimental <i>Desmodesmus subspicatus</i> (Green algae) DIN 38412 L9; Static Reduced growth rate observed
	(b) 72 h NOEC = 0.07 mg/L (c) 72 h NOEC = 3.4 mg/L (d) 72 h NOEC = 0.97 mg/L	Experimental <i>Pseudokirchneriella subcapitata</i> (Green algae) OECD TG 201 Reduced growth rate observed

Effects on Sediment-Dwelling Life

Bioavailable forms of lead(2+) are very toxic to sediment-dwelling organisms.

Toxicity of lead(2+)

The toxicity of lead to sediment-dwelling organisms has been summarised in the rationale and background information to the Australian and New Zealand Guidelines for Fresh and Marine Water Quality. Exposure to sediment contaminants for benthic organisms is assumed to principally involve pore waters (ANZECC, 2000b). The available NOEC value equivalents for select sediment-dwelling organisms (corrected to a CaCO₃ concentration of 30 mg/L) include a NOEC of 5.1 micrograms of lead per litre (µg Pb/L) for the amphipod *Gammarus pseudolimnaeus* and a NOEC of 28 µg Pb/L for the midge *Tanytarsus dissimilis* (ANZECC, 2000a). However, toxicity is highly dependent on sediment chemistry, which is complex and depends on a range of variable environmental parameters such as dissolved oxygen, pH and the geochemistry of sediment particles (ANZECC, 2000b). In particular, the presence of natural organic matter and the formation of sulfides will affect lead bioavailability. These factors must also be considered when determining the toxicity of lead(2+) to sediment-dwelling species.

Toxicity of medium-chain fatty acids

No suitable data were available to evaluate the effects of the fatty acid constituents of these chemicals on sediment-dwelling organisms. However, the release of lead(2+) ions to the sediment compartment is expected to dominate ecotoxicity concerns for these salts.

Effects on Terrestrial Life

Bioavailable forms of lead(2+) are toxic to terrestrial organisms.

Toxicity of lead(2+)

The toxicity of lead to terrestrial organisms has been summarised in Schedule B5c of the *National Environment Protection (Assessment of Site Contamination) Measure 1999* (Cwlth). Lead is strongly adsorbed to organic matter in soil and therefore bioavailability is typically limited. Mean NOEC values for terrestrial invertebrates range from 129 milligrams of lead per kilogram of soil (mg Pb/kg soil) for the earthworm *Dendrobaena rubida* to 1797 mg Pb/kg soil for the springtail *Fautrix candida*. Plants are also susceptible to lead toxicity, with mean NOEC values in a range from 50 mg Pb/kg soil for barley (*Hordeum vulgare*) to 546 mg Pb/kg soil for the Loblolly pine (*Pinus taeda*). Reproductive toxicity and impaired growth are listed as the most common toxic effects (Commonwealth of Australia, 1999).

Toxicity of medium-chain fatty acids

Limited data are available in regards to the toxicity of medium chain fatty acids to terrestrial organisms. The toxicity of lauric acid is low, with dietary LC50 values greater than 5620 mg/L available for the birds *Colinus virginianus* and *Anas platyrhynchos*, and low-observed effect level (LOEC) values for a variety of mosquitoes (*Culex* sp.) ranging from 64.1 mg/L to 200 mg/L. No-observed effect level (NOEL) values for mosquitoes (*Aedes aegypti* and *Culex* sp.) ranging from 14.4 mg/L to 46.1 mg/L were also available for octanoic acid (LMC, 2013).

Predicted No-Effect Concentration (PNEC)

The primary environmental effects of the chemicals in this group are expected to be caused by the release of lead(2+) ions.

In place of the PNECs for aquatic and sediment compartments for this ionic component, the trigger values published for lead in the Australian and New Zealand Guidelines for Fresh and Marine Water Quality have been used. These values represent thresholds above which further assessment of potential toxicity may be required to ensure environmental quality. Although they were not developed for risk assessment purposes, they nevertheless provide important reference values for evaluating the risks posed by anthropogenic emissions of lead to the Australian environment. For freshwater ecosystems with low water hardness (30 mg/L CaCO₃), a high reliability trigger value for protection of 95% of species has been determined to be 3.4 µg Pb/L. The equivalent value for protection of marine species is 4.4 µg Pb/L. For the sediment compartment, the trigger value is 50 mg Pb/kg, dry weight (ANZECC, 2000c).

In place of a PNEC for the soil compartment for lead(2+), the added contaminant limit published for lead in the *National Environment Protection (Assessment of Site Contamination) Measure 1999* (Cwlth) has been used. This value represents the level above which further investigation or evaluation is required after considering naturally occurring background levels. For soil where the contaminant has been present for less than two years, the contaminant limit for protection of 99% of species is 110 mg added Pb/kg soil (Commonwealth of Australia, 1999).

Categorisation of Environmental Hazard

It is not currently possible to categorise the environmental hazards of metals and other inorganic chemicals according to standard persistence, bioaccumulation and toxicity (PBT) hazard criteria. These criteria were developed for organic chemicals and do not take into account the unique properties of inorganic substances and their behaviour in the environment and biota (UNECE, 2007; US EPA, 2007). Therefore, environmental hazard categorisation according to domestic PBT criteria has only been performed for the organic components of the chemicals in the Lead Salts of Medium-Chain Carboxylic Acids group, as presented below.

Persistence

Lead neodecanoate

Persistent (P). Based on the low biodegradation observed in a ready biodegradability study of the component acids, the organic components of lead neodecanoate are categorised as Persistent.

All remaining chemicals

Not Persistent (Not P). Based on results obtained from various biodegradation studies which indicate rapid and ultimate biodegradation of straight-chain and iso-branched medium-chain fatty acids, the organic components of all chemicals in this group, except lead neodecanoate, are categorised as Not Persistent.

Bioaccumulation

Not Bioaccumulative (Not B). Based on the results of a bioconcentration study for neodecanoic acid and the essential biological functions of medium-chain fatty acids as dietary fats and the associated homeostatic controls, the organic components of all chemicals in this group are categorised as Not Bioaccumulative.

Toxicity

Lead octanoate

Toxic (T). Based on the available chronic ecotoxicity value for algae, the organic component of lead octanoate is categorised as Toxic.

All remaining chemicals

Not Toxic (Not T). Based on available acute ecotoxicity values greater than 1 mg/L, and chronic ecotoxicity values greater than 0.1 mg/L, the organic components of all chemicals in this group except for lead octanoate are categorised as Not Toxic.

Summary

The organic component of octanoic acid, lead salt is categorised as:

- Not P
- Not B
- T

The organic components of neodecanoic acid, lead salt are categorised as:

- P
- Not B
- Not T

The organic components of isooctanoic acid, lead salt; isononanoic acid, lead salt; decanoic acid, lead salt; dodecanoic acid, lead salt; and hexanoic acid, 2-ethyl-, lead salt are all categorised as:

- Not P
- Not B
- Not T

An environmental hazard categorisation for the inorganic lead component of the chemicals in this group has not been assigned for the reasons discussed above. Nevertheless, there is an international consensus that bioavailable forms of lead are highly toxic to the environment and that lead bioaccumulates in most organisms (UNEP, 2010; 2014).

Risk Characterisation

Risk quotients (RQs) have not been calculated for these chemicals.

The chemicals in this group contain lead(2+) ions, which can be released into the environment from industrial applications. Anthropogenic emissions of lead to the environment are acknowledged to be of concern, both domestically and internationally, due to the bioaccumulation properties and high toxicity of bioavailable forms of lead. Environmental contamination by lead is of particular concern because high exposure to lead compounds can cause neurological defects and reproductive toxicity across a range of organisms, including humans, plants and animals (UNEP, 2010; 2014).

However, the release of lead to the environment in Australia from industrial uses of chemicals in this group is expected to be limited in volume and diffuse in nature. Available use data suggests that the contribution of lead from current industrial uses of lead salts of medium-chain fatty acids to total environmental lead loads is comparatively small. Domestic restrictions regarding lead content in surface coatings and international trends to reduce lead in paint have dramatically reduced the consumption of these lead salts for their main industrial use as driers in coatings.

Key Findings

The main industrial use of chemicals in the Lead Salts of Medium-Chain Carboxylic Acids group is expected to be in industrial coatings. Many chemicals in this group have previously been used in paints and other coating products internationally. However, available information from domestic and international sources indicates that the use of lead salts of medium-chain fatty acids in these products has largely been phased out.

The principal environmental concern for industrial uses of lead salts of medium-chain fatty acids is the potential for release of soluble forms of ionic lead from articles on which industrial coatings have been used. This poses a concern because lead and lead compounds are considered to be highly significant environmental contaminants. However, the potential for lead to be released to the environment due to current use of the chemicals in this group in paints and other coating products is expected to be greatly reduced compared to historic emissions.

The chemicals in this group are considered to pose a low and declining risk to the environment based on the expected limited contribution to total anthropogenic lead emissions from current uses of industrial coating products containing lead based driers. This main use has been phased out. No further assessment of the environmental risks of these chemicals is currently required.

The organic components of the chemicals in the Lead Salts of Medium-Chain Carboxylic Acids group are not PBT substances according to domestic environmental hazard criteria.

Recommendations

The seven chemicals in the Lead Salts of Medium-Chain Carboxylic Acids 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 octanoic acid, lead salt; isooctanoic acid, lead salt; isononanoic acid, lead salt; decanoic acid, lead salt; neodecanoic acid, lead salt; dodecanoic acid, lead salt; and hexanoic acid, 2-ethyl-, lead salt according to the third edition of the United Nations' Globally Harmonised System of Classification and Labelling of Chemicals (GHS) is presented below (UNECE, 2009):

Hazard	GHS Classification (Code)	Hazard Statement
Acute Aquatic	Category 1 (H400)	Very toxic to aquatic life
Chronic Aquatic	Category 1 (H410)	Very toxic to aquatic life with long lasting effects

The classification of octanoic acid, lead salt; decanoic acid, lead salt and dodecanoic acid, lead salt (lead laurate) was conducted based on the water solubility data available for the 1:2 lead(2+) salts of these acids as obtained from the studies conducted by Hunter and Liss (1976) and Mauchauffee et al. (2008), and the ecotoxicological data identified in this assessment (ECHA, 2014a; LMC, 2013). These chemicals are classified as Acute Aquatic Category 1 as the calculated maximum lead(2+) ion concentrations at saturation for the stoichiometric lead(2+) salts exceed all acute toxicity values for lead identified in this assessment for aquatic species. Based on this classification, and the global consensus that lead bioaccumulates in aquatic organisms, these chemicals are also classified as Chronic Aquatic Category 1 according the GHS classification strategy for metals and metal compounds (UNECE, 2007). While these chemicals may contain components beside the stoichiometric lead(2+) salts, the values obtained for the 1:2 lead(2+) salts are considered appropriate for read-across to determine the potential for the chemicals in this group to release lead(2+) ions into the aquatic environment.

Based on the available K_{sp} values, and the observed trend in solubility for metal soaps, hexanoic acid, 2-ethyl, lead salt; isononanoic acid, lead salt; isooctanoic acid, lead salt and neodecanoic acid, lead salt are considered to be of equal or greater solubility than lead laurate. Therefore, these chemicals will be considered more toxic than lead laurate under the GHS. However, lead laurate has been classified under the highest environmental hazard categories available. Therefore, these more soluble chemicals have been classified under the same aquatic hazard categories as lead laurate.

It is preferable to classify the hazard posed by metals and metal compounds using the findings of a study conducted in accordance with the OECD Transformation and Dissolution protocol (UNECE, 2007). Therefore, should a study conducted in accordance with this protocol suggest a lower hazard classification is warranted, these chemicals may be reclassified as appropriate.

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