TRISODIUM CITRATE

This dossier on trisodium citrate presents the most critical studies pertinent to the risk assessment of trisodium citrate in its use in coal seam gas extraction activities. It does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the OECD-SIDS documents on citric acid (OECD 2001a,b) and the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Trisodium citrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Trisodium citrate is readily biodegradable and is not expected to bioaccumulate. Trisodium citrate is the sodium salt of citric acid. This compound can be referred to as simply sodium citrate, though sodium citrate can refer to any of the three trisodium salts of citric acid (namely trisodium citrate, trisodium citrate dihydrate and trisodium citrate pentahydrate). Trisodium citrate is highly soluble and is expected to be fully dissociated to citrate and sodium ions in water and therefore is unlikely to adsorb to soil or sediment. Trisodium citrate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Trisodium 2-hydroxypropane-1,2,3-tricarboxylate

CAS RN: 68-04-2

Molecular formula: $C_6H_5Na_3O_7$

Molecular weight: 258.06 g/mol

Synonyms: Sodium citrate; trisodium 2-hydroxypropane-1,2,3-tricarboxylate; 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, trisodium salt

3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

Table 1 Overview of the Physico-chemical Properties of Trisodium Citrate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Crystalline solid	2	ECHA
Melting Point	>150°C (pressure not reported)	2	ECHA
Boiling Point	Not available; decomposition	-	ECHA

Property	Value	Klimisch score	Reference
Density	1,857 kg/m^3 @ 20°C	2	ECHA
Vapour Pressure	Negligible @ 25°C	2	ECHA
Partition Coefficient (log K_{ow})	-0.2 to -1.8 for citric acid (temperature not provided)	4	ECHA
Water Solubility	@ 400 – 700 g/L @ 20-25 °C	4	ECHA
Dissociation constant (pKa)	3.13, 4.76, 6.4 @ 25 °C for citric acid	2	ECHA

4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns were identified within Australia and internationally for trisodium citrate.

NICNAS has assessed trisodium citrate in an IMAP Tier 1 assessment and concluded that it poses no unreasonable risk to human health or the environment[1] .

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

5 ENVIRONMENTAL FATE SUMMARY

A. Summary

Trisodium citrate is readily biodegradable. It is not expected to bioaccumulate. Trisodium citrate is highly soluble and is expected to be fully dissociated to citric acid/citrate and sodium ions in water and therefore is unlikely to adsorb to soil or sediment.

[1] https://www.industrialchemicals.gov.au/chemical-information/search-assessments?assessmentcasnumber=68-04-2

B. Partitioning

Trisodium citrate lacks any of the functional group that are susceptible to hydrolysis in aqueous solution.

C. Biodegradation

Trisodium citrate dissociates in aqueous solutions to sodium (Na^+) and citrate ($C_6H_5O_7^-$) ions. Trisodium citrate can be considered readily biodegradable based on the results of the ready and inherent aerobic biodegradation studies on citric acid/citrate listed in Table 3.

If a chemical is found to be inherently or readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

Table 3 Biodegradation Studies on Citric Acid (OECD 2001a,b)

Test System	Results*	Notes	Klimisch Score
Modified Sturm	97% (CO_2 evolution); 100% (DOC removal)	Readily biodegradable; exposure period not stated	2
Closed Bottle Test	BOD_{30}/COD Ratio = 90%	Readily biodegradable	2
BOD_5/COD Ratio	BOD_5 = 526 mg; COD = 728 mg; BOD_5/COD Ratio = 0.72	Readily biodegradable; concentration of test substance and activated sludge not stated	2
BOD_1/ThOD Ratio	BOD_1/ThOD Ratio = 13%	-	2
BOD_{20}/ThOD Ratio	BOD_{20}/COD Ratio = 98%	Readily biodegradable; initial test substance concentration 720 mg/L	2
Zahn-Wallen Test	85%, 1 day (DOC removal)	Inherently biodegradable	2
Zahn-Wallen Test	98%, 7 days (DOC removal)	Inherently biodegradable	
Coupled Units Test	93% (COD removal)	Ultimately biodegradable; exposure period not stated	2

D. Environmental Distribution

No experimental data are available for trisodium citrate or citric acid. Using KOCWIN program in EPISuite™ (USEPA, 2016), the estimated soil organic carbon partition coefficient (K_{oc}) value for citric acid from the octanol/water partition coefficient (K_{ow}) value of -1.08 is 0.3617 L/kg.

If released to soil, based on this negligible K_{oc} value, this substance is unlikely to adsorb to soil and would be highly mobile. If released to water, based on a negative K_{ow} value and high water solubility, this substance is unlikely to adsorb to suspended solids and would preferentially partition to the water column.

E. Bioaccumulation

The log K_{ow} for trisodium citrate is very low and falls between -0.2 to -1.8. Thus, trisodium citrate is not expected to bioaccumulate.

As noted above, trisodium citrate dissociates in aqueous solution to the metal ion (Na^+) and citrate ions ($H_7C_6O_7^-$). Citrate is found in all eukaryotic cells as an intermediate of the Tricarboxylic acid (TCA) cycle, which is part of the basic metabolic pathway that generates useable energy from carbohydrates, proteins and fats. Citric acid is formed and broken down in the course of this cycle at very high rates (ECHA).

An estimated BCF for citric acid was 3.2 L/kg (ECHA) [Kl. Score = 2]. The weight of evidence of the low estimated BCF, biodegradability and role in cell metabolism indicate that citric acid is extremely unlikely to bioaccumulate (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Trisodium citrate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

No reliable data is available assessing the toxicity of trisodium citrate to fish or algae, however, data for the parent compound, citric acid, is available. Table 4 lists the results of acute aquatic toxicity studies conducted on citric acid (CAS No. 77-92-9).

Table 4 Acute Aquatic Toxicity Studies on Trisodium Citrate*

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Leuciscus idus melanotus (golden orfe)	48-hr LC_{50}	590	2	ECHA
Daphnia magna	48-hr EC_{50}	2,055	2	ECHA

*Value based on citric acid converted to trisodium citrate using a factor of 1.34 (ECHA)

In addition, the 8-day toxicity threshold value (EC_0) for citric acid in *Scenedesmus quadricauda* is 640 mg/L, from which a NOEC value of 425 mg/L (citric acid) was derived. However the algal study should not be considered due to the essential nutrient complexing properties of the test substance that do not permit to assess the true toxicity of the test substance (ECHA). [Kl. Score = 2].

Chronic Studies

No studies are available. As outlined in ECHA, testing is not considered necessary because:

- Short-term toxicity to aquatic organisms is low.
- Risk characterisation ratios based on $PNEC_{aquatic}$ calculated using the short-term data are <1.

- The parent acid substance is naturally occurring in aquatic organisms and so is the counter ion.

C. Terrestrial Toxicity

No studies are available. The substance has a negative log K_{ow} value and therefore, partitioning to the terrestrial compartment is expected to be minimal (ECHA).

7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN

A. PBT Categorisation

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (InCHEMS,2022; ECHA, 2017).

Trisodium citrate is readily or inherently biodegradable; thus, it does not meet the screening criteria for persistence.

The log K_{ow} values for trisodium citrate is between -0.2 and -1.8. Thus, trisodium citrate does not meet the screening criteria for bioaccumulation.

There are no chronic aquatic toxicity studies on citric acid or trisodium citrate. The acute $E(L)C_{50}$ values for citric acid are >1 mg/L in fish and invertebrates. Thus, it does not meet the screening criteria for toxicity.

The overall conclusion is that trisodium citrate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for trisodium citrate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment [1]	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required[3]
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity [2]	Chronic Toxicity[2]	
Trisodium Citrate	68-04-2	Not a PBT	No	No	No	No	No	No	1	No Data	1

Footnotes:

1 - PBT Assessment based on PBT Framework.

2 - Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra. Available: www.environment.gov.au/water/coal-and-coal-seam-gas/national-assessment-chemicals/consultation-risk-assessment-guidance-manual

ECHA. ECHA REACH database: https://echa.europa.eu/information-on-chemicals/registered-substances

European Chemicals Agency [ECHA]. (2017). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland. Available: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment

Industrial Chemicals Environmental Management Standard [IChEMS]. (2022). Australian Environmental Criteria for Persistent, Bioaccumulative and/or Toxic Chemicals. Available: https://www.dcceew.gov.au/sites/default/files/documents/australian-pbt-criteria.pdf

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

OECD. (2001a). IUCLID Data Set for Citric acid (CAS No. 77-92-9), UNEP Publications.

OECD. (2001b). Screening Information Dataset (SIDS) Initial Assessment Report for Citric acid (CAS No. 77-92-9), UNEP Publications).

USEPA. (2016). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BOD	biological oxygen demand
COC	constituent of concern
COD	chemical oxygen demand
DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency

EU	European Union
g/L	grams per litre
IChEMS	Industrial Chemicals Environmental Management Standard
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
mg	milligrams
mg/L	milligrams per litre
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TCA	tricarboxylic acid
ThOD	theoretical oxygen demand
USEPA	United States Environmental Protection Agency