

NITRILOTRIACETIC ACID, TRISODIUM SALT MONOHYDRATE

This dossier on nitrilotriacetic acid, trisodium salt monohydrate presents the most critical studies pertinent to the risk assessment of nitrilotriacetic acid, trisodium salt monohydrate in its use in their use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from 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 – Nitrilotriacetic acid, trisodium salt monohydrate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Nitrilotriacetic acid, trisodium salt monohydrate (Na₃NTA) is an organic sodium salt composed of sodium and nitrilotriacetate ions in a 3:1 ratio. Na₃NTA dissociate to form a common moiety, nitrilotriacetate ion. The substance is used to soften water and to remove traces of heavy metals. It is also commonly used as chelating and sequestering agents, and as builders in detergent and cleaning formulations for domestic and commercial use.

Na₃NTA is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil. It exhibits low toxicity to aquatic and terrestrial organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): trisodium-2-[bis(carboxymethyl)amino]acetate

CAS RN: 5064-31-3

Molecular formula: C₆H₉NO₆.3Na

Molecular weight: 257.08 g/mol

Synonyms: Trisodium nitrilotriacetate; glycine, N,N-bis(carboxymethyl)-,trisodium salt; trisodium 2,2',2''-nitrilotriacetate; Nitrilo triacetic acid, 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 Na₃NTA

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	2	ECHA
Melting Point	340°C (decomposes) (pressure not provided)	2	ECHA

Property	Value	Klimisch score	Reference
Boiling Point	No data as the substance is a solid which melts above 300°C	-	ECHA
Density	1770 kg/m ³ @ 20°C	2	ECHA
Vapour Pressure	-	-	ECHA
Partition Coefficient (log K _{ow})	-13.2 @ 25°C	2	ECHA
Water Solubility	457 g/L @ 20°C	2	ECHA
Viscosity	Not applicable	-	ECHA
Dissociation constant	1.22 @ 25°C	2	ECHA

Since sodium salts are generally considered to be completely dissociating, a solution of Na₃NTA in water yields the tribasic anion nitrilotriacetate. Na₃NTA is a weak acid, and in such a solution, the NTA will therefore exist as an equilibrium mixture of several species:



with the last species occurring when, in a very acidic environment, the central nitrogen atom is protonated (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 nitrilotriacetic acid, trisodium salt monohydrate.

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

Na₃NTA is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil.

B. Biodegradation

Na₃NTA was tested for ready biodegradability according to OECD 301 E (BASF, 1983b,c), OECD 301 F (in addition to a combined CO₂/DOC test, see Strotmann et al., 1995), and Sturm Test (BASF, 1983d), and in a die away test (Takahashi et al, 1997) as well as for inherent biodegradability according to OECD 302 B (BASF, 1983a). These tests resulted in 75 -100 % degradation after 7 to 28 days with lag phases ranging between 1 and 16 days. According to results from ready biodegradation tests, Na₃NTA can be regarded as readily biodegradable (ECHA) [KI. Score = 2].

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

C. Environmental Distribution

A relevant adsorption of Na₃NTA onto the organic fraction of soils, sediments or suspended solids is not expected due to the ionic structure of the substance and a log K_{ow} of -13.2 (pH 7). However, interaction with the mineral phase may be possible (ECHA) [KI. Score = 2]. Based on its low log K_{ow} and high water solubility values, if released to soil, Na₃NTA is expected to have low potential for adsorption and a high potential for mobility. If released to water, it is likely to remain in water and not adsorb to sediment.

D. Bioaccumulation

There are no bioaccumulation studies on Na₃NTA. Bioaccumulation of Na₃NTA is not expected to occur because of its log K_{ow} of -13.2 at pH 7, is highly water-soluble, and is unlikely, due to its polar nature, to be taken up by fish gills or across other biological membranes (ECHA).

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Na₃NTA exhibits low toxicity to aquatic and terrestrial organisms. Details are provided below.

B. Aquatic Toxicity

Acute Studies

Table 3 presents the results of acute aquatic toxicity studies on Na₃NTA.

Table 3 Acute Aquatic Toxicity Studies on Na₃NTA

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Pimephales promelas</i>	96-hour LC ₅₀	103	2	ECHA
<i>Gammarus pseudolimnaeus</i>	96-hour LC ₅₀	80	2	ECHA
<i>Scenedesmus subspicatus</i>	72-hour EC ₅₀	>91.5	1	ECHA

Other data were deemed as less reliable; and, as a result, are not shown in Table 3.

Chronic Studies

In a 32-week fish (*Pimephales promelas*) chronic study, the measured NOEC values \geq 54 mg/L (ECHA). [Kl. score = 2]. In a 27-day fish (*Oncorhynchus mykiss*) chronic study, the measured LC₅₀ value for 50 mg/L hardness was 90.5 mg/L and for 200 mg/L hardness was 114 mg/L (ECHA) [Kl. Score = 2].

In a 21-week *Gammarus pseudolimnaeus* reproduction study, the measured NOEC value was 9.3 mg/L (ECHA). [Kl. score = 2].

In a 21-day *Daphnia* reproduction study, the measured NOEC value was 100 mg/L for survival and reproduction (ECHA). [Kl. score = 3]

In a 120-day *Helisoma trivolvis* reproduction study, the measured NOEC value was 12.5 mg/L for growth (ECHA) [Kl. Score = 2].

C. Terrestrial Toxicity

There are no ecotoxicity studies for terrestrial organisms relating to Na₃NTA. It is reasonable to assume that trends seen in aquatic toxicity are likely to be observed in terrestrial organisms. These short- and long-term aquatic data, when considered with bioaccumulative and degradation information, result in Na₃NTA being practically non-toxic to aquatic organisms. It is reasonable to assume that Na₃NTA will also be non-toxic to soil organisms (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 (DEWHA, 2009; ECHA, 2008).

Na₃NTA is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of -13.2, Na_3NTA does not meet the screening criteria for bioaccumulation.

The lowest chronic EC_{10} or NOEC value for Na_3NTA is >0.1 mg/L. The acute EC_{50} values are >1 mg/L. Thus, Na_3NTA does not meet the criteria for toxicity.

The overall conclusion is that Na_3NTA is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for Na_3NTA .

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	
Nitilotriacetic acid, trisodium salt monohydrate	5064-31-3	Not a PBT	No	No	No	No	No	No	1	1	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, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

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.

ECHA. ECHA REACH database: <http://echa.europa.eu/information-on-chemicals/registered-substances>

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

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.

B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
hPa	hectopascal
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
MCI	molecular connectivity index
mg/L	milligrams per litre
mPa s	millipascal second
NOEC	no observed effect concentration
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases