TETRAMETHYLAMMONIUM CHLORIDE

This dossier on tetramethylammonium chloride (TMAC) presents the most critical studies pertinent to the risk assessment of TMAC in its use in hydraulic fracturing fluids. 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 – TMAC was assessed as a tier 1 chemical for acute toxicity. This was based on aquatic toxicity studies for TMAC in fish along with the preponderance of data for read-across substance tetramethylammonium hydroxide (TMAOH) in invertebrates and algae indicating a classification of tier 1 (3 of 4 studies). TMAC was assessed as a tier 3 chemical for chronic toxicity based on a single aquatic toxicity study for TMAC in invertebrates. However, TMAC is determined to biodegrade in the environment very quickly suggesting chronic lab data would be less relevant than acute results. As a result, based on preponderance of data and biodegradation information, TMAC is classified overall as a **Tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

No biodegradation studies are available on TMAC; however, it is expected to be readily biodegradable based on tetramethylammonium hydroxide studies. TMAC has a moderate potential for adsorption to soil. It is not expected to bioaccumulate based on an octanol water partition coefficient (log Know) of <0.027. TMAC and its surrogate tetramethylammonium hydroxide (TMAOH) have moderate acute toxicity and high chronic toxicity concern for aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): N,N,N-trimethylmethanaminium chloride

CAS RN: 75-57-0

Molecular formula: $C_4H_{12}ClN$ or $(CH_3)_4NCl$

Molecular weight: 109.6 g/mol

Synonyms: Tetramethylammonium chloride; N,N,N-trimethylmethanaminium chloride; TMAC; tetramethylazanium; chloride

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 Tetramethylammonium chloride

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White hydroscopic powder with large solid lumps.	2	ECHA
Melting Point	268°C @ 101.3 kPa	1	ECHA
Boiling Point	Decomposition at 300°C before boiling point	1	ECHA
Density	1190 kg/m^3 @ 20°C	1	ECHA
Vapour Pressure	<1.6 x 10^{-8} Pa @ 25°C	1	ECHA
Partition Coefficient (log K_{ow})	-1.6 @20°C	1	ECHA
Water Solubility	>1,000 g/L @ 20°C (pH 3.6)	1	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 TMAC.

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

No biodegradation studies are available on TMAC; however, it is expected to be readily biodegradable based on TMAOH studies. TMAC has a moderate potential for adsorption to soil. It is not expected to bioaccumulate based on a log K_{ow} of <0.027.

B. Partitioning

TMAC is a quaternary ammonium salt, indicating that this compound will exist in the cation form in the environment and cations generally adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts. As a salt, volatilisation from water or moist soil surfaces is not expected to be an important fate process. Likewise, based on its vapour pressure, volatilisation of TMAC from dry surfaces is also not expected to be an important fate process (PubChem).

Hydrolysis is not expected to be an important environmental fate process since this compound is a quaternary ammonium salt (PubChem).

C. Biodegradation

No biodegradation studies are available on TMAC. A 25% aqueous solution of TMAOH, a surrogate for TMAC, was readily biodegradable in an OECD 301B test. Degradation was 84% and 100% after 14 and 25 days, respectively (ECHA) [Kl. score = 1]. A 27.5% aqueous solution of TMAOH was readily biodegradable in an OECD 301C test. There was >90% degradation within 14 days (ECHA) [Kl. score = 2]. TMAOH was also readily biodegradable by adapted sludge under anaerobic conditions (ECHA) [Kl. 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).

D. Environmental Distribution

TMAC was tested in three different types of soil: loamy sand, sandy loam and clay soil. The mean K_{oc} for the three soils was 546 L/kg (ECHA). [Kl. score = 1]

If released to soil, based on this K_{oc} value, TMAC has a moderate potential for adsorption to soil. If released to water, based on this K_{oc} value along with its high water solubility, it is expected to also have a moderate potential for adsorption to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on TMAC. TMAC is not expected to bioaccumulate based on a log K_{ow} of <0.027 (ECHA) [Kl. score = 1].

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

TMAC and its surrogate TMAOH have moderate acute toxicity and high chronic toxicity concern for aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on TMAC and its surrogate TMAOH.

Table 3 Acute Aquatic Toxicity Studies on TMAC and its surrogate TMAOH

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Pimephales promelas	96-hr LC_{50}	462	2	ECHA
Daphnia magna	48-hr EC_{50}	3.6*	2	ECHA
Daphnia magna	48-hr EC_{50}	16.6*	2	ECHA
Pseudokirchneriella subcapitata	72-hr EC_{50}	115*	2	ECHA
Desmodesmus subspicatus	72-hr EC_{50}	>301*	2	ECHA

*Test substance was TMAOH; values adjusted for TMAC (TMAC/TMAOH = 109/91).

Chronic Studies

An 11-day *Daphnia* reproduction study was conducted on TMAC. The NOEC was 0.03 mg/L (ECHA). [Kl. score = 2]

C. Terrestrial Toxicity

No studies are available.

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).

TMAC is expected to be readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on a measured log K_{ow} of <0.027, TMAC does not meet the screening criteria for bioaccumulation.

The lowest NOEC from the chronic aquatic toxicity studies on TMAC is <0.1 mg/L. Thus, TMAC does meet the criteria for toxicity.

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

B. Other Characteristics of Concern

No other characteristics of concern were identified for TMAC.

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]	
Tetramethylammonium chloride	75-57-0	Not a PBT	No	No	No	No	No	Yes	1	3	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:

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.

PubChem. PubChem open chemistry database: https://pubchem.ncbi.nlm.nih.gov

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
IUPAC	International Union of Pure and Applied Chemistry
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration

mg/L	milligrams per litre
NOEC	no observed effects concentration
OECD	Organisation for Economic Co-operation and Development
Pa	Pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
TMAC	tetramethylammonium chloride
TMAOH	tetramethylammonium hydroxide