SODIUM ACETATE

This dossier on sodium acetate presents the most critical studies pertinent to the risk assessment of sodium acetate in its use in coal seam gas extraction activities. This dossier 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 – Sodium acetate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium acetate is the salt of acetic acid, and acetic acid is widely used in the coal seam gas industry as a pH adjuster and for iron control (DoEE, 2017a).

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. Both of these chemical species are naturally occurring and ubiquitous in the aquatic environment. The acetate ion is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment. The acetate ion is of low acute toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium acetate

CAS RN: 127-09-3

Molecular formula: $C_2H_4O_2.Na$

Molecular weight: 82.03 g/mol

Synonyms: Acetic acid, sodium salt, Sodium acetate anhydrous, Acetic acid sodium 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 Sodium Acetate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	crystalline or white granular powder	1	ECHA
Melting Point	324 °C @ 101.3 kPa	1	ECHA
Boiling Point	Not applicable as substance is solid.	-	ECHA
Density	1530 kg/m^3 @ 20 °C	1	ECHA

Property	Value	Klimisch score	Reference
Vapour pressure	Not applicable	-	ECHA
Partition Coefficient (log P_{ow})	-3.72	2	ECHA
Water Solubility	1,250 g/L @ 25 °C	1	ECHA
Dissociation Constant (pKa)	4.756	4	ECHA

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. Acetate is ubiquitous in natural water and acts as a key nutrient, supplying energy to heterotrophic algae under aerobic conditions. Acetate is also formed by anaerobic bacteria through natural fermentation processes as a source of energy. Sodium ions are similarly naturally ubiquitous in the environment (DoEE, 2017a).

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 sodium acetate.

Based on an assessment of hazards, NICNAS identified the substance as a chemical of low concern to human health and the environment (NICNAS, 2017 and DoEE, 2017b). Chemicals of low concern are considered to have a low likelihood of causing adverse human health effects should an exposure occur and are unlikely to have adverse environmental effects if they are released to the environment from coal seam gas operations.

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

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. Both of these chemical species are naturally occurring and ubiquitous in the aquatic environment. The acetate ion is readily biodegradable, is not expected to bioaccumulate, and has a low potential to adsorb to soil or sediment.

B. Partitioning

Sodium acetate disassociates in water to form sodium ions (Na+) and acetate ($H_3C2O_2^-$) ions. The pKa of sodium acetate (as acetic acid) is 4.76, indicating that this substance will exist partially in anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts (PubChem).

C. Biodegradation

The substance is considered readily degradable. The biodegradability was determined with a non adapted activated sludge for the test item over a test period of 28 days in the DOC-Die-Away test. At 7 days, the biodegradation reached the 86% and at 28 days the biodegradation reached the 99% (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, 2017b).

D. Environmental Distribution

No experimental data are available for sodium acetate. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} values from log K_{ow} is 1.0 L/kg (ECHA) [KI. Score = 2]. Based on this value, sodium acetate has a low potential for adsorption to soil and sediment and is expected to have very high mobility in soil.

Release of large volumes of sodium acetate (or acetic acid) to natural waterways may disturb the health of aquatic ecosystems through direct and indirect physical and chemical effects. For example, at very high concentrations, these chemicals have the potential to modify the pH beyond normal ranges. Further, rapid biodegradation of large quantities of these chemicals in natural water bodies may decrease dissolved oxygen concentrations to levels which are insufficient to sustain normal respiration by aquatic life. However, numerous natural biogeochemical mechanisms exist which tend to limit fluctuations in nutrient levels, which occur frequently in healthy aquatic ecosystems. (DoEE, 2017a).

E. Bioaccumulation

There are no reliable bioaccumulation studies on sodium acetate. The low Log K_{ow} (-3.72) suggests sodum acetate will not bioaccumulate to a substantial degree ((ECHA)[KI Score = 2].

Further, bioaccumulation of sodium acetate is not expected to occur because the substance dissociates completely in aqueous solution to acetate and its sodium ion. Both ions are ubiquitous in the environment. Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

The acetate ion is of low acute toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute

The aquatic toxicity data for sodium acetate are presented in Table 3.

Table 3. Acute Aquatic Toxicity Studies on Sodium Acetate

Test Species	Endpoint	Results (mg/L)	Klimisch Score	Reference
Brachydanio rerio	96h-LC50	> 100 mg/L	2	ECHA
Daphnia magna	EC50 (48h)	>385.60	2	ECHA
Acartia tonsa	LC50 (48h)	2075.20	2	ECHA
Algae and cyanobacteria (unspecified)[1]	EC50 (unspecified duration)	417.92	2	ECHA

1 – testing read across from potassium acetate

Chronic Studies

No chronic data are available.

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).

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

Bioaccumulation of sodium acetate is not expected to occur because the substance dissociates completely in aqueous media to acetate and its sodium ion. Both ions are ubiquitous in the environment. Acetate is naturally found in eukaryotic and prokaryotic cells and is involved in their biochemical pathways. The log K_{ow} for sodium acetate is -3.72. Thus, sodium acetate does not meet the screening criteria for bioaccumulation.

The acute toxicity values for tested species are all > 1mg/L. Thus, sodium acetate does not meet the screening criteria for toxicity.

There are no chronic toxicity studies on sodium acetate. The acute E(L)C_{50} values were greater than 1 mg/L. Thus, sodium acetate does not meet the criteria for toxicity.

The overall conclusion is that sodium acetate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium acetate

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]	
Sodium acetate	127-09-3	Not a PBT	No	No	No	No	No	No	1	No data available	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). 2017b. Environmental risks associated with surface handling of chemicals used in coal seam gas extraction in Australia, Project report prepared by the Chemicals and Biotechnology Assessments Section (CBAS), in the Chemicals and Waste Branch of the Department of the Environment and Energy as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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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.

NICNAS. 2017. Chemicals of low concern for human health based on an initial assessment of hazards, Project report prepared by the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) as part of the National Assessment of Chemicals Associated with Coal Seam Gas Extraction in Australia, Commonwealth of Australia, Canberra.

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
IUPAC	International Union of Pure and Applied Chemistry

kPa	kilopascal
LC	lethal concentration
mg/L	milligrams per litre
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent Bioaccumulative Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
ThOD	Theoretical oxygen demand