DISODIUM OCTABORATE TETRAHYDRATE

This dossier presents the most critical studies pertinent to the risk assessment of disodium octaborate tetrahydrate 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 –Disodium octaborate tetrahydrate is classified as a tier 1 chemical and requires a hazard assessment only.

1. BACKGROUND

Disodium octaborate tetrahydrate is a boron compound. Boron compounds (including boron oxides, boric acid, boron minerals) have a wide range of applications in industry (e.g. manufacture of glass, fibreglass and porcelain enamels, and precursors for chemical manufacture), agriculture (e.g. fertilisers, herbicides and insecticides), and in household settings (e.g. flame retardants and detergents) and personal care products. Borate salts are commonly used in coal seam gas applications internationally (NICNAS, 2019).

Disodium octaborate tetrahydrate as a natural element is not degradable. It is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

Disodium octaborate tetrahydrate has low acute and chronic toxicity to aquatic organisms.

2. CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): disodium octaborate

CAS RN: 12008-41-2

Molecular formula: \( \text{Na}_2\text{B}_8\text{O}_{13} \cdot 4\text{H}_2\text{O} \)

Molecular weight: 412.4 g/mol

Synonyms: boron sodium oxide tetrahydrate; boric acid, disodium salt, tetrahydrate; disodium octaborate tetrahydrate

3. PHYSICAL AND CHEMICAL PROPERTIES

Key physical and chemical properties for disodium octaborate tetrahydrate are shown in Table 1.
Table 1: Overview of the Physico-chemical Properties of Disodium Octaborate Tetrahydrate

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Klimisch score</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state at 20°C and 101.3 kPa</td>
<td>White, odorless, crystalline powder</td>
<td>1</td>
<td>ECHA</td>
</tr>
<tr>
<td>Melting Point</td>
<td>&gt;1,000°C (pressure not provided)</td>
<td>1</td>
<td>ECHA</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>Not Applicable</td>
<td>-</td>
<td>ECHA</td>
</tr>
<tr>
<td>Density</td>
<td>1874 kg/m³ @ 20°C</td>
<td>1</td>
<td>ECHA</td>
</tr>
<tr>
<td>Vapor Pressure</td>
<td>9.9 x 10⁻¹⁷ Pa @ 25°C</td>
<td>1</td>
<td>ECHA</td>
</tr>
<tr>
<td>Partition Coefficient (log K_{ow})</td>
<td>Not Applicable, substance is inorganic</td>
<td>-</td>
<td>ECHA</td>
</tr>
<tr>
<td>Water Solubility</td>
<td>223.65 g/L @ 20°C</td>
<td>1</td>
<td>ECHA</td>
</tr>
<tr>
<td>Dissociation Constant (pKa)</td>
<td>8.94 @ 20°C</td>
<td>1</td>
<td>ECHA</td>
</tr>
</tbody>
</table>

Boron is almost exclusively found in the environment in the form of boron-oxygen compounds, which are often referred to as borates. The high strength of the B-O bond relative to those between boron and other elements makes boron oxide compounds stable compared to nearly all non-oxide boron materials. Indeed, the B-O bond is among the strongest found in the chemistry of naturally occurring inorganic substances (ECHA).

In the environment, the chemicals in this group will dissociate and/or hydrolyse to release boron as boric acid [B(OH) (also formulated as H BO₃)] and/or borate anions (NICNAS, 2019).

Exposure to borates are often expressed in terms of boron (B) equivalents based on the fraction of boron in the source substance on a molecular weight basis. The B equivalents used are a generic designation rather than a designation of the element boron. The factor for converting disodium octaborate tetrahydrate to B-equivalents is 0.2096.

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 disodium octaborate tetrahydrate.
Table 2  Existing International Controls

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

5. ENVIRONMENTAL FATE PROPERTIES

A. Summary

Disodium octaborate tetrahydrate as a natural element is not degradable. It is highly soluble in water. Some partitioning to soil and sediment does occur, but this adsorption is pH dependent. It has a low potential for bioaccumulation.

B. Partitioning

Chemicals in this group will transform into boric acid in the aquatic environment. In the environment boric acid is in equilibrium with borate anions. Both species are very stable as they do not undergo biotransformation or redox reactions under normal environmental conditions. Boric acid is highly water soluble and it tends to remain in surface waters. Although some partitioning from water to soil and sediment does occur, the adsorption is pH dependent with the greatest adsorption occurring under alkaline conditions (pH 7.5 to 9.0) (NICNAS, 2019).

C. Biodegradation

Degradation is not applicable to inorganic borates, such as disodium octaborate tetrahydrate. It is not subject to hydrolysis, photodegradation, or biodegradation (ECHA). Inorganic borates are subject to chemical transformation processes (adsorption, complexation, precipitation, fixation) once released into the environment (ECHA).

D. Environmental Distribution

The Kp value for disodium octaborate tetrahydrate was calculated as the median of all measured Kp values from the GEMAS project (Geochemical Mapping of Agricultural and Grazing Land Soil project): 2.19 L/kg dry weight (ECHA) [KI. Score = 2]. The chemistry of boron in soils and aquatic systems is simplified by the absence of oxidation-reduction reactions or volatilization. Redox processes can mobilize Fe oxides and Mn oxides, which may lead to a release of boron in aquatic systems. Generally, sediments are characterised with higher pH values than the soil matrix, which increases the boron sorption capacity (ECHA).

If released to soil, based on this low Kp value, low vapour pressure and high water solubility, disodium octaborate tetrahydrate is considered relatively mobile in the environment, under certain conditions (ECHA).
E. Bioaccumulation

The WHO review of boron (WHO, 1998) noted that “highly water soluble materials are unlikely to bioaccumulate to any significant degree and that borate species are all present essentially as undissociated and highly soluble boric acid at neutral pH”. A BCF of <0.1 was reported in Chinook salmon fed boron-supplemented diets for 60 to 90 days (Hamilton and Wiedmeyer, 1990).

6. ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Disodium octaborate tetrahydrate has low acute and chronic toxicity to aquatic organisms.

B. Aquatic Toxicity

In ecotoxicological tests for boron, the exposure concentrations are expressed as boron equivalents i.e. mg B/L. This is because boric acid and borate salts will have the same boron speciation when dissolved in environmental matrices. Therefore, in the following sections toxicological values are given as mg B/L regardless of the form of boron that was tested.

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on disodium octaborate tetrahydrate.

<table>
<thead>
<tr>
<th>Test Species</th>
<th>Endpoint</th>
<th>Results (mg/L)</th>
<th>Klimisch score</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fathead minnow</td>
<td>96-hr LC50</td>
<td>79.7</td>
<td>2</td>
<td>ECHA</td>
</tr>
<tr>
<td>Stonefly, Shortwing snowfly</td>
<td>96-hr LC50</td>
<td>476</td>
<td>2</td>
<td>ECHA</td>
</tr>
<tr>
<td>Pseudokirchneriella subcapitata</td>
<td>72-hr EC50</td>
<td>52.4 mg B/L</td>
<td>1</td>
<td>ECHA</td>
</tr>
</tbody>
</table>

Chronic Studies

Long-term effects (LC10) on freshwater fish ranged from 3.5 to 47 mg B/L. Adequate long-term LC10 of 21.6 mg B/L was found for the fresh water fish *P. promelas* in a study according to EPA OPPTS 850.1400 (ECHA) [Kl. Score = 2].

Long-term effects (LC10/NOEC) on reproduction on freshwater vertebrates ranged from 6.6 to 32 mg B/L based on several well-accepted guideline studies (ECHA) [Kl. Scores =1 or 2].

Boric acid has been evaluated for its toxicity towards the fresh water alga *Pseudokirchneriella subcapitata* (formerly *Selenastrum capricornutum*) in an Alga growth inhibition test according to OECD 201 under GLP requirements. The exposure duration was 72 hours under static conditions. The NOEC growth rate determined from the study was 17.5 mg B/L (ECHA) [Kl. Score = 1].
The ANZG water quality guideline (2021) derived a very high reliability default guideline value (DGVs) for (dissolved) boron in freshwater from 22 chronic (long-term) toxicity data, comprising eight fish, two amphibians, three crustaceans, one bivalve, three macrophytes, one green microalga, three diatoms and one blue–green alga. The summary of representative data used by ANZG to develop a water quality guideline for boron is presented in Table 5 below. These values are noted to be consistent with those reported in ECHA. Additional chronic aquatic toxicity data is found in the ANZG Technical Brief (ANZG, 2021).

**Table 5: Chronic Aquatic Toxicity Studies on Boron**

<table>
<thead>
<tr>
<th>Test Species</th>
<th>Endpoint</th>
<th>Results (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Danio rerio</td>
<td>34-day NOEC (Biomass)</td>
<td>1.8</td>
</tr>
<tr>
<td>Pimephales promelas</td>
<td>32-day NOEC (Mortality)</td>
<td>11</td>
</tr>
<tr>
<td>Daphnia magna</td>
<td>14-day NOEC (Reproduction)</td>
<td>2.4</td>
</tr>
<tr>
<td>Pseudokirchneriella subcapitata</td>
<td>4-day NOEC (Growth)</td>
<td>2.8</td>
</tr>
</tbody>
</table>

1 - The DGVs are based on toxicity data for boron as either boric acid, H$_3$BO$_3$ (CAS 10043-35-3), or borax, Na$_2$B$_4$O$_7$·10H$_2$O (CAS 1303-96-4), in freshwater.

In the chronic toxicity data set, fish sensitivity to boron ranged from the least sensitive species in the dataset (*Melanotaenia splendida*, LC10 102 mg/L) to the third most sensitive species in the dataset (*Danio rerio*, NOEC 1.8 mg/L). Of the crustaceans, *D. magna* was best represented in the literature, with 18 published NOEC values (ranging from 2.4 mg/L to 29 mg/L) for six different endpoints from six different publications. The final NOEC of 2.4 mg/L used in the DGV derivation was lower than that for *C. dubia* (NOEC 5.6 mg/L) and for the amphipod *H. azteca* (NOEC 6.6 mg/L). For *P. subcapitata*, there were three separate studies available with toxicity data for boron. The toxicity values from these studies ranged from a NOEC of 2.8 mg/L to a NEC of 27 mg/L, varying with endpoint, duration and test medium used. Boron was least toxic to *P. subcapitata* when tested in algal growth medium with added NaHCO$_3$, suggesting that carbonate addition may have influenced boron toxicity. Therefore, although NECs are preferred to NOECs or EC10s (Warne et al. 2018), in this instance, a reliable NOEC of 2.8 mg/L was the most sensitive toxicity value for *P. subcapitata* (ANZG, 2021).

**C. Terrestrial Toxicity**

Ecotoxicological tests with plants and soil invertebrates have recorded modest chronic toxicity values (NOECs/ECs) in the range of 15.3 to 84.0 and 5.2 to 315 mg total B/kg, respectively (ECHA, 2008). However, to predict the potential toxicity of boron to plants and soil organisms, measuring the total boron concentration may be unsuitable. Instead, potential toxicity is better predicted using boron concentrations in the soil solution (extractable boron) (Mertens et al., 2011). In Australia, it is generally accepted that boron toxicity will pose a risk to terrestrial plants when soil concentrations exceed 15 mg/kg of extractable boron (NICNAS, 2019).

The avian toxicity studies conducted on disodium octaborate and boric acid are presented in Table 6.
Table 6: Avian Toxicity Studies on Disodium Octaborate and Boric Acid

<table>
<thead>
<tr>
<th>Test Species</th>
<th>Test Substance</th>
<th>Endpoint</th>
<th>Results</th>
<th>Klimisch score</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mallard duck</td>
<td>Disodium octaborate</td>
<td>dietary LC₅₀</td>
<td>&gt;2,100 mg B/kg food</td>
<td>1</td>
<td>EU, 2007</td>
</tr>
<tr>
<td>Bobwhite quail</td>
<td>Boric acid</td>
<td>dietary LC₅₀</td>
<td>&gt;983 mg B/kg food</td>
<td>1</td>
<td>EU, 2007</td>
</tr>
<tr>
<td>Bobwhite quail</td>
<td>Disodium octaborate</td>
<td>Oral gavage LD₅₀</td>
<td>&gt;527 mg B/kg bw</td>
<td>4</td>
<td>EU, 2007</td>
</tr>
<tr>
<td>Bobwhite quail</td>
<td>Disodium octaborate</td>
<td>dietary LC₅₀</td>
<td>&gt;2,100 mg B/kg food</td>
<td>1</td>
<td>EU, 2007</td>
</tr>
</tbody>
</table>

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).

Disodium octaborate tetrahydrate is an inorganic compound that dissociates completely to boric acid and the borate anion in aqueous media. Biodegradation is not applicable to these inorganic compounds; both boric acid and borate are also ubiquitous and are present in most water, soil and sediment. For the purposes of this PBT assessment, the persistent criteria are not considered applicable to disodium octaborate tetrahydrate.

Disodium octaborate tetrahydrate is a water-soluble substance that is not expected to bioaccumulate. Limited data indicate that bioaccumulation (BCF values are low) is not significant in aquatic and terrestrial food chains. Thus, it does not meet the criteria for bioaccumulation.

The chronic toxicity data on disodium octaborate tetrahydrate has a NOEC > 0.1 mg/L. Thus, disodium octaborate tetrahydrate does not meet the criteria for toxicity.

The overall conclusion is that disodium octaborate tetrahydrate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for disodium octaborate tetrahydrate.
### SCREENING ASSESSMENT

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>CAS No.</th>
<th>Overall PBT Assessment</th>
<th>Chemical Databases of Concern Assessment Step</th>
<th>Persistence Assessment Step</th>
<th>Bioaccumulative Assessment Step</th>
<th>Toxicity Assessment Step</th>
<th>Risk Assessment Actions Required</th>
</tr>
</thead>
<tbody>
<tr>
<td>Disodium Octaborate Tetrahydrate</td>
<td>12008-41-2</td>
<td>Not a PBT</td>
<td>Listed as a COC on relevant databases?</td>
<td>Identified as Polymer of Low Concern</td>
<td>P criteria fulfilled?</td>
<td>Other P Concerns</td>
<td>B criteria fulfilled?</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>No</td>
<td>No</td>
<td>NA</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

**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


B. Abbreviations and Acronyms

°C degrees Celsius
AICS Australian Inventory of Chemical Substances
ANZG Australian and New Zealand Guidelines
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  kilograms
Kl  Klimisch scoring system
KOCWIN™  USEPA organic carbon partition coefficient estimation model
kPa  kilopascal
L  litre
L/kg  litres per kilogram
LC  lethal concentration
LD  lethal dose
LOAEL  lowest observed adverse effect level
m³  cubic metre
MCI  molecular connectivity index
mg/kg  milligrams per kilogram
mg/L  milligrammes per litre
mg/m³  milligrams per cubic metre
mL  millilitre
mPa s  millipascal second
NICNAS  The National Industrial Chemicals Notification and Assessment Scheme
NOAEL  no observed adverse effect level
NOEC  no observed effect concentration
NEC  no effect concentration
Pa  pascal
PBT  Persistent, Bioaccumulative and Toxic
ppm  parts per million
REACH  Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD  Reference Dose
SGG  Synthetic Greenhouse Gases
USEPA  United States Environmental Protection Agency