Document III-A: Study Summaries - Active Substance Disodium Octaborate Tetrahydrate

Section A1 Applicant

Annex Point IIA1

1.1	**Applicant**	**Lead Notifier: Rio Tinto Minerals** Contact: [redacted] 2 Eastbourne Terrace London, W2 6LG United Kingdom [redacted] **Website: www.riotinto.com** **Joint Notifier: Societa Chimica Larderello spa** Contact: [redacted] Via Fara 28 I-20124 Milan ITALY [redacted] **Administrative Consortium Lead** Dr Roger Doome c/o European Borates Association (EBA) [redacted] Please correct the email address to r.doome@ima-europe.eu *Email: r.doome@ima-eu.org*	Official use only
1.2	**Manufacturer of Active Substance** (if different)	Borates for Biocidal use are manufactured in the USA US Borax Inc 14486 Borax Road Boron, CA 93516-2000 USA *Tel: + 1 760 762 7000* **Joint Notifier: Societa Chimica Larderello spa** As Above	X1
1.3	**Manufacturer of Product(s) (if different)**	*As above*	

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 1.2, Manufacturer
	For US Borax Inc the whole address is changed
Manufacturer	Borates for Biocidal use are manufactured in the USA
	US Borax Inc
	14486 Borax Road
	Boron, CA 93516-2000
	USA
	Tel: + 1 760 762 7000
Reliability	-
Acceptability	acceptable
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Document III-A: Study Summaries - Active Substance Disodium Octaborate Tetrahydrate

Section A2 Identity of Active Substance

Subsection (Annex Point)			Official use only
2.1	Common name (IIA2.1)	Disodium octaborate tetrahydrate Sodium octaborate; Boron sodium oxide (B8Na2O12) tetrahydrate; Boric acid (H2B8O13), disodium salt, tetrahydrate; Boric acid, disodium salt, tetrahydrate; DOT; Various trade names including POLYBOR, TIMBOR, SOLUBOR; DOT; Foliael	X1
2.2	Chemical name (IIA2.2)	Disodium octaborate tetrahydrate; Boron sodium oxide (B8Na2O13), tetrahydrate or Boric acid (H2B8O13), disodium salt, tetrahydrate	X2
2.3	Manufacturer´s development code number(s) (IIA2.3)	Not relevant	
2.4	CAS No and EC numbers (IIA2.4)		X3
2.4.1	CAS-No	12280-03-4	
2.4.2	EC-No	234-541-0	
2.4.3	Other	Not relevant	
2.5	Molecular and structural formula, molecular mass (IIA2.5)	Non-entry field	
2.5.1	Molecular formula	$Na_2B_8O_{13}.4H_2O$	
2.5.2	Structural formula	$B_8H_8O_{17}Na_2$ Disodium octaborate tetrahydrate is a solid solution of boric acid and disodium tetraborate decahydrate. It breaks down to these components in aqueous solutions and therefore can be considered to exist as undissociated boric acid under physiological conditions. The structures of both boric acid and disodium tetraborate decahydrate in their respective IUCLID files	X4
2.5.3	Molecular mass	412.52	
2.6	Method of manufacture of the active substance (IIA2.1)	[redacted]	X5

Section A2 Identity of Active Substance

2.7 Specification of the purity of the active substance, as appropriate (IIA2.7)

g/kg | g/l | % w/w >99% | % v/v

X6

Borax Europe Ltd:

Disodium Octaborate Tetrahydrate	% w/w	
	B2O3	**Purity**
Typical	67.0	99.2
Maximum	68.6	102.2
Minimum	66.0	97.5

Societa Chimica Larderello spa:

Disodium Octaborate Tetrahydrate	% w/w	
	B2O3	**Purity**
Typical	67.4	99.9
Maximum	68.9	102.1
Minimum	67.3	99.7

2.9 The origin of the natural active substance or the precursor(s) of the active substance (IIA2.9)

Natural inorganic mineral ore

Borax Europe Limited: Ores
Tincal ($Na_2O.2B_2O_3.10H_2O$)
Kernite ($Na_2O.2B_2O_3.4H_2O$)

X7

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	1-Feb-2005
Materials and methods	Section 2.1. Common name
	Common name should be discerned from synonyms and trade names
Conclusion	common name: disodium octaborate tetrahydrate
	synonyms: sodium octaborate; boron sodium oxide tetrahydrate; boric acid disodium salt tetrahydrate; DOT;
	trade names: POLYBOR, TIMBOR, SOLUBOR; Foliarel, Borowood
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	1-Feb-2005
Materials and methods	Section 2.2. Chemical name The RMS prefers disodium octaborate tetrahydrate as chemical name.
Conclusion	chemical name: disodium octaborate tetrahydrate
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and Methods	Section 2.4 CAS number and EC number. On the ECB website only one CAS number was found for disodium octaborate: * disodium octaborate anhydrous, CAS no 12008-41-2, EC no 234-541-0. Therefore two CAS numbers exist for the same compound.
Conclusion	Two CAS numbers exist for the same compound. * Disodium octaborate tetrahydrate, CAS no 12280-03-4 * Disodium octaborate anhydrous, CAS no 12008-41-2 For this CA-report, CAS no is 12280-03-4 is used (tetrahydrate form). CAS no 12008-41-2 is only used for the anhydrous form and is not assessed in this CA-report. EC number 234-541-0 is assigned to both disodium octaborate tetrahydrate and disodium octaborate anhydrous. In this CA-report only disodium octaborate tetrahydrate is assessed.
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	21-Feb-05
Materials and methods	Section 2.5.2. Structural formula. The a..s is an amorphous mixture of boric acid and disodium tetraborate dechydrate/pentahydrate and therefore a structural formula cannot be established.
Conclusion	No data available; not required.
Reliability	-
Acceptability	Acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	1-Feb-05
Materials and methods	Section 2.6: Manufacturing process a. The manufacturing process is considered as an industrial scale process, although this is not indicated by the notifier. b. There are two notifiers and only one manufacturing process is described. The manufacturing process described is the manufacturing process for Borax Europe Ltd. The manufacturing process for Societa Chimica Larderello spa (SCL) is classified as confidential. The description of the process is given schematically in a separate appendix, indicated as Doc IIIA (2.6 and 2.9) SCL.
Conclusion	as indicated by the notifier.
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 2.7: Purity of active substance a. The specification data cannot be verified by the RMS, because batch analyses are not submitted. These are however not required. b. A disodium octaborate tetrahydrate purity higher than 100% is not possible. c. Another frequently used formula for disodium octaborate tetrahydrate is $Na_2O.4B_2O_3.4H_2O$. Based on this formula the purity can also be expressed as B_2O_3-content. In this case 67-69% B_2O_3. It is not useful to express the content as boric oxide, because this compound as such is not present in disodium octaborate tetrahydrate. The formula suggests that disodium octaborate tetrahydrate is boric oxide with added crystallisation water and added sodium oxide, which is not correct. Both boric oxide, sodium oxide and water are not present in disodium octaborate tetrahydrate. d. The purity is indicated as >99%. But in the specification table the minimum purity for Borax Europe Ltd is given as 97.5%. Therefore minimum purity should be 97.5%. e. The minimum purity data for the Societa Larderello spa product (99.7%) do not comply with the purity of the active substance used in tests for physical chemical properties (see IIIA3.1.1, IIIA3.1.3, IIIA3.4, IIIA3.5). In these tests the minimum purity was 98%.
Conclusion	Based on impurity data and tests with the active substance, the minimum purity specification proposed by the RMS is 97.5% (w/w) expressed as $Na_2B_8O_{13}.4H_2O$ for both manufacturers.
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	1-Feb-05
Materials and methods	Section 2.9: Origin of natural active substance The origin of natural active substance of Societa Chimica Larderello spa is classified as confidential. The origin is given in a separate appendix, indicated as Doc IIIA (2.6 and 2.9) SCL.
Conclusion	as indicated by the notifier
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Document III-A: Study Summaries - Active Substance Disodium Octaborate Tetrahydrate

Section A2.8 Identity of impurities and additives (active substance)

Annex Point IIA2.8 *fill in one form for each impurity/additive*

X1

2.8 Identity of impurities and additives, as appropriate (IIA2.8)

Borax Europe Ltd:

Trace quantities of boric acid (CAS No. 10043-35-3) borax (CAS No. 1330-43-4) and water plus typical levels of:

Disodium Octaborate Tetrahydrate	% w/w		
	Fe	Cl	SO_4
Typical	0.0010	0.0150	0.0400

The impurities listed are not controlled in the production process and therefore there are no maximum guarantees for these impurities in this product. Variation in the purity and impurities is also due to the degree of hydration of boric oxide. This variable is dependant on the manufacturing process. Therefore water will be the difference up to 100%.

Societa Chimica Larderello spa:

	Fe	Cl	SO_4	Insolubles in water
Typical	5ppm	10ppm	50ppm	40ppm

2.8.1 Isomeric composition Not relevant

2.8.1.1 Common name

2.8.1.2 Function Not relevant

2.8.2 IUPAC name

2.8.3 CAS-No

2.8.4 EC-No

2.8.5 Other

2.8.6 Molecular formula

2.8.7 Structural formula

2.8.8 Molecular mass *Give molecular mass in g/mol*

2.8.9 Concentration of the impurity or additive g/kg g/l % w/w % v/v

RMS, Section A2.8	**Identity of impurities and additives (active substance)**
Annex Point IIA2.8	*fill in one form for each impurity/additive*
RMS 2.8.1 Common name and function	non-entry field
RMS 2.8.1.1. Common name	traces of iron, chlorine, sulphate boric acid, disodium tetraborate anhydrous.
RMS 2.8.1.1. Function	impurity of starting material
RMS 2.8.2 IUPAC name	not applicable
RMS 2.8.3 CAS no	Fe, not applicable Cl, not applicable SO_4, not applicable boric acid, 10043-35-3 disodium tetraborate anhydrous, 1330-43-4 CRC Handbook of Chemistry and Physics, 1999
RMS 2.8.4 EC no	not applicable for Fe, Cl, SO_4 boric acid, 233-139-2 disodium tetraborate anhydrous, 215-540-4
RMS 2.8.5 Other	not applicable
RMS 2.8.6 Molecular formula	Fe, Cl, SO_4 boric acid: general formula H_3BO_3, other frequently used formulas are $B(OH)_3$ and $B_2O_3.3H_2O$. disodium tetraborate anhydrous: general formula $Na_2B_2O_7$, other frequently used formula $Na_2O.2B_2O_3$ (water free).
RMS 2.8.7 Structural formula	unknown
RMS 2.8.8 Molecular mass	Fe = 55.845 Cl = 35.4527 SO_4 = 32.066(6) + 4x 15.9994(3) = 96.043 boric acid = 61.833 disodium tetraborate anhydrous = 201.22 Reference: CRC Handbook of Chemistry and Physics, 1999
RMS 2.8.9 Concentration of impurity or additive *typical and range of concentrations*	**Borax Europe Ltd:** Trace quantities of boric acid, disodium tetraborate anhydrous and water plus typical levels of:

Disodium Octaborate Tetrahydrate	**% w/w**		
	Fe	**Cl**	**SO_4**
Typical	0.0010	0.0150	0.0400

The impurities listed are not controlled in the production process and therefore there are no maximum guarantees for these impurities in this product. Variation in the purity and impurities is also due to the degree of hydration of boric oxide. This variable is dependant on the manufacturing process. Therefore water will be the difference up to 100%.

Societa Chimica Larderello spa:

	Fe	**Cl**	**SO_4**	**Insolubles in water**
Typical	5ppm	10ppm	50ppm	40ppm

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 2.8 Identity of impurities a. The summary written by the notifier is not according to template. Therefore the whole section was rewritten by the RMS. b. It is assumed that 1 ppm = 1 mg/kg or 0.0001% w/w. c. The specification data for impurities cannot be verified by the RMS, because batch analyses are not submitted. These are, however, not required. d. Although the typical concentrations for Fe, Cl and SO_4 are stated, no minimum and maximum concentrations are given. Typical concentrations of boric acid and disodium tetraborate anhydrous are not given at all. The notifier indicates that impurities are not controlled during the process and that therefore no range of impurities can be given. e. The impurities for the Borax Europe product add up to 0.056 % (w/w), while the Societa Chimica Larderello product adds up to 0.0055 % (w/w). Impurities are compliable with the minimum purity of 97.5% as proposed by the RMS (see section IIIA2.7).
Conclusion	Maximum specified impurities are compliable with the minimum purity of 97.5% (w/w) expressed as $Na_2B_8O_{13}.4H_2O$ as proposed by the RMS.
Reliability	-
Acceptability	acceptable
Remarks	
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Document III-A: Study Summaries - Active Substance Disodium Octaborate Tetrahydrate

Section A2.10
Annex Point IIA2.10

Exposure data in conformity with Annex VIIA to Council Directive 92/32/EEC (OJ No L, 05.06.1992, p. 1) amending Council Directive 67/548/EEC

Subsection			Official use only
2.10.1	**Human exposure towards active substance**	In the occupational exposure measurements of borates it is preferential to determine the boron value of the sample and to equate this to individual borates where appropriate. The basis for this is due to a number of factors. 1. Borates are susceptible to weight change due to uptake or loss of water and this hydration instability can lead to gravimetric and interpretation errors in field samples. 2. There may be a mix of borates in the sample and borate species cannot be easily characterised by chemical analysis. 3. Boron can be measured to a high level of accuracy. Therefore assessment of all borates is covered in Doc IIIA Boric Acid REF: *Smith, R.A.; Ascherl, F.M Issues concerning the measurement of borate in occupational environments. Am. Ind. Hyg. Assoc. J.,* 60, *No. 5, p.651-658. (September - October 1999)*	
2.10.1.1	**Production**	See Doc III A Boric Acid	
2.10.1.2	**Intended use(s)**	Wood Preservation Professional (Industrial and Professional) and Non Professional (Amateur Use) use The simple inorganic borates such as boric acid; boric oxide; disodium tetraborate and disodium octaborate tetrahydrate are used for wood preservation formulations depending upon requirements such as pH, total solubility, solubility rate, compatibility with other substances in the formulation, etc. They are primarily used in solution where they are completely dissolved. All formulations will be designed to give an efficacious level of boric acid in the wood to comply with various Standards of Wood preservation (so need to supply a specific boric acid level). Once the borate is in solution and the wood is treated, the risk assessment of the wood will be the same regardless of the starting material at Mixing and Loading Stage. Therefore the Exposure data is the same regardless of the borate staring material and is all presented in the Boric Acid Dossier Doc IIIA & B	
2.10.2	**Environmental exposure towards active substance**	Releases to the environment are measured in terms of boron and are covered in Doc IIIA Boric Acid	
2.10.2.1	**Production**	See Doc IIIA Boric Acid	

2.10.1.2 Intended use(s)	Emissions to the environment will be the same species of borate (boric acid). In solution, borates form a variety of polymeric species derived from monomeric boric acid, $B(OH)_3$. The presence of these species is dependent upon solution pH and concentration. It has been shown for solutions of boric acid and sodium borates below pH 8 and at a solution concentration of below 0.1M, the borate is present as boric acid. This has been borne out in an independent study aimed at identifying the species present in systems under typical biologically active conditions, i.e. pH 6.5-pH7.5 and <0.02M. Raman spectroscopy confirmed the presence of $B(OH)_3$ as the species present. The pH or soils and rain is typically in the range 6-8 and therefore the borate leached from timber which is present at low concentration will be $B(OH)_3$.

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	3-Oct-05
Materials and methods	Section IIIA2.10 Human exposure assessment a. In Doc. II B Exposure Assessment for the Biocidal Product' the exposure assessment is described in section 8. Background information about the processes and values are described in Doc. III A2.10. The exposure calculation was not given, it was received from the notifier via the Board for the Authorization of Pesticides (Mail EBA, 11-05-05). b. To calculate the dermal exposure during mixing and loading and during application the notifier used the 'dermal absorption flux'. The dermal exposure was calculated by multiplying this flux (in mg/(cm^2 x hour)) with the total body surface area and with the exposure duration. The flux is derived from a dermal absorption study in volunteers (see Doc IIIA6.2). The flux (µg / (cm^2 x hour)) which is calculated here for the different active substances (a.s.), is a measure for the quantities of the different a.s. absorbed by the skin in the test concerned. This flux is a measure for the amount absorbed by the skin. However, in the exposure calculation during mixing and loading and application, it is used as measure for the amount of active substance deposited on the skin. This is not correct. Environmental exposure assessment c. Upon evaluation, the main input (use classes under consideration, dosages and leaching rates) as used in the applicant's assessment appeared to be either not relevant, incorrect or inconsistent. Therefore, RMS conducted a new environmental exposure assessment according to the OECD Emission Scenario Document for Wood preservatives. The reader is therefore referred to the environmental exposure assessment as performed by RMS, which is included in Doc IIB, Sections 3.3 and following subsections.
Conclusion	Human exposure assessment In our view, the approach in which the notifier has calculated the exposure is not correct. The calculations are therefore not provided with annotations. The exposure can be calculated by means of the models mentioned in the TNsG (2002). In the User Guidance TNsG (2002), the human exposure to wood preservatives is extensively described; to calculate the exposure to wood

	preservatives the most appropriate models and its parameter values are stated. The exposure to borates is calculated by using the selected models and default values for wood preservatives from the User Guidance TNsG (2002) as a guideline. Via the Board for Authorization of Pesticides (CTB) the proposal to the notifier was to calculate the exposure with this approach in addition to their own method. The notifier has done these calculations likewise (mail EBA, 09-05-05). In Doc IIB, section 3 'Exposure Assessment' the calculations which we have done are reported. In the calculations the process information given by the notifier is used as base for the calculations. Where the calculations differ from the notifier's calculations, this is mentioned. Environmental exposure assessment The above presented exposure assessment of the applicant is not considered correct. The reader is therefore referred to the environmental exposure assessment as performed by RMS, which is included in Doc IIB, Sections 8.3 and following subsections.
Reliability	3
Acceptability	Not acceptable
Remarks	

	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Document III-A: Study Summaries - Active Substance Disodium Octaborate Tetrahydrate

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results Give also data on test pressure, temperature, pH and concentration range if necessary	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point	-	-	-	Disodium octaborate tetrahydrate is not a true compound but a solid solution of borax (CAS No. 1330-43-4) in boric acid (CAS No. 10043-35-3). Its formula approximates to $Na_2B_8O_{13}.4H_2O$.	-	2	Mellor's Comprehesive Treatise on Inorganic & Theoretical Chemistry, Volume V Boron, Part A: Boron-Oxygen Compounds, Longman, London and New York, 1980.	X1
Melting pt. 1	Thermal gravimetric analysis method.	98%	**result:** 815°C	The value reported was determined in the Borax Groups own laboratory using Thermal gravimetric analysis.	N	2	-	
Melting pt. 2	ASTM E 537-76 (Differential Thermal Analysis)	98%	**result:** No melting point detected below 1000°C. **pressure:** Atmospheric Temperature range: 25 to 1000°C.	A small exothermal effect was observed at 567/567°C. This effect is possibly caused by the phase transition of the amorphous to the crystalline sodium pentaborate. An endothermal effect was observed at 813/803°C. This effect is not a clear melting peak. It could represent the melting of anhydrous sodium pentaborate (literature value 785°C).	Y	1	Cordia J.A. [redacted] 2003,	

Section A3 Physical and Chemical Properties of Active Substance

3.1.2 Boiling point	-	-	-	Not applicable since the product will lose water of crystallisation on heating from around 100°C and becomes fully anhydrous at approx. 500°C and finally melts at approx. 815°C. Anhydrous forms of sodium tetraborates start to decompose at 1575°C giving Na_2O and B_2O_3. Boric oxide (B_2O_3) has a boiling point of 2200°C.	-	2	-	X2
3.1.3 Bulk density/ relative density								X3
Bulk/rel. density 1	-	-	Bulk density: 320-480 kg m^{-3}.	-	N	2	Technical data sheet EC14, issued by Borax Consolidated Ltd., London, UK.	
Bulk/rel. density 2	Test Guideline A.3 of EC Directive 92/69/EEC and TNO-PML Standard Operation Procedure Q211-W-030. A multi-volume pyncnometer was used.	98%	Relative density: 1.874 ± 0.009 at 22 ± 1°C	-	Y	1	Cordia J.A. [redacted] 2003,	
3.2 Vapour pressure (IIA3.2)								X4
Vapour pressure 1	Directive 84/449/EEC A.4.	~99%	**temperature:** 25°C **result:** <9.9 x 10^{-11} hPa	The vapour pressure of disodium octaborate tetrahydrate is negligible at ambient temperature.	Y	1	Howard R.. [redacted] 1995.	

Section A3 Physical and Chemical Properties of Active Substance

3.2.1 Henry´s Law Constant (Pt. I-A3.2)	-	-	-	Not applicable to materials of low vapour pressure. Disodium octaborate tetrahydrate is a solid substance.	-	-	-	X5
3.3 Appearance (IIA3.3)								X6
3.3.1 Physical state			Solid					
3.3.2 Colour			White					
3.3.3 Odour			Odourless					
3.4 Absorption spectra (IIA3.4)								X7
UV/VIS	OECD Guideline 101 and TNO-PML S.O.P. Q213-W-058.	98%	The molar extinction coefficient could not be determined.	No unusual effects were observed in running the spectra. The molar extinction coefficient of the test substance could not be determined because there were no district absorption maximum or minimum found in a netural, basic or acidic medium.	Y	1	Cordia J.A. [redacted] 2003,	
IR	TNO-PML S.O.P. Q214-W-125 version 2.	98%	Peaks observed at 696 and 785 cm^{-1}.	The sample was ground in KBr powder and pressed. The test substance was recorded on and FTIR-spectrometer.	Y	1	Cordia J.A. [redacted] 2003,	
NMR	-	-	-	The recording of the ^{13}C NMR Spectrum of the test substance as reflected in TNO protocol no. 014.16566 dated August 23, 2004 is irrelevant due to the fact that the test substance does not contain carbon atoms.	Y	1	Spruit [redacted] 2005,	

Section A3 Physical and Chemical Properties of Active Substance

MS	TNO-PML S.O.P. Q214-W-130.	98%	No signals characteristic of borium containing material.	A broad range of experimental conditions was used: positive and negative ions, variation of the cone voltage, variation of the flow-injection eluent and dissolution of the compounds in water or eluent. No signals produced characteristic of borium containing material.	Y	1	Cordia J.A. [redacted] 2003,	
3.5 Solubility in water (IIA3.5) Water Solubility	Test Guideline A.6 of EC Directive 92/69/EEC and TNO-PML S.O.P. Q213-W-036.	98%	**result:** 95 g/l **temperature:** 20°C **pH:** 8.5 **result:** 223.65 ± 6.73 g/l **temperature:** 20.0 ± 0.5°C. **pH:** 7.64 ± 0.01	The solubility of DOT is difficult to give precisely because the material supersaturates. Supersaturation is a condition in which the solvent (water) contains more dissolved matter (solute, or in this case, DOT) than is present in a saturated solution of the same material at an equivalent temperature. Solubilities of 223.65 ± 6.73 g/l have been reported (Cordia et al) for supersaturated solutions. These solutions are unstable. A more practical approach is to consider the concentration of DOT remaining in solution, following precipitation of a supersaturated solution, which is 95 g/l. The solution pH decreases as the concentration increases	Y		Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & sons Inc., 1992, 4th Edition, Volume 4, page 384-386. Cordia J.A. [redacted] 2003,	X8
3.6 Dissociation constant (-)	-	-	Not required.	*Only if additional data are required (see BPD, TNsG)*	-	-	-	X9

Section A3 Physical and Chemical Properties of Active Substance

3.7	**Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)**	-	-	No data.	*Only if additional data are required (see BPD, TNsG)*	-	-	-	X10
3.8	**Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)**	-	-	Not required.	*Only if additional data are required (see BPD, TNsG)*	-	-	-	X11
3.9	**Partition coefficient n-octanol/water (IIA3.6)**	-	-	-	The partition coefficient of disodium octaborate tetrahydrate cannot be measured because of substantial conversion of all sodium borates into undissociated boric acid in aqueous solution. Disodium octaborate is a solid solution of boric acid and disodium tetraborate decahydrate. It breaks down to these components in aqueous solutions and therefore can be considered to exist as undissociated boric acid under physiological conditions. Refer to boric acid (CAS No. 10043-35-3) and disodium tetraborates (CAS No. 1330-43-4).	No data	2	Barres M., Rev. Chim. Miner., 1967, 4, 803-838.	X12
3.10	**Thermal stability, identity of relevant breakdown products (IIA3.7)**	-	-	-	Loss of water on heating, otherwise thermally stable to 815°C minimum (see melting point).	-	-	-	X13

Section A3 Physical and Chemical Properties of Active Substance

3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	-	-	Not applicable.	Disodium octaborate tetrahydrate is a non-volatile, non-flammable inorganic solid. The product is used as a flame retardant. Product has been classified according to 29 CFR 1910.1200 as a non-flammable solid.	-	-	-	X14
3.12 Flash-point (IIA3.9)	-	-	Not applicable.	Disodium octaborate tetrahydrate is a non-volatile, non-flammable inorganic solid. The product is used as a flame retardant.	-	-	-	
3.13 Surface tension (IIA3.10)								X15
Surface tension 1	-	-	No data	Refer to borax tetraborate pentahydrate physico- chemical properties.	-	-	-	
3.14 Viscosity (-)	-	-	Not applicable.	Solid substance to ≥815°C.	-	-	-	
3.15 Explosive properties (IIA3.11)	-	-	-	Potential explosive properties are indicated by the presence of certain reactive groups in the molecule. The molecular structure of none of the substances indicates that such groups are present. No reactive or instable groups are present. The molecular structure does not indicate that these substances will explode under the conditions of the test as described in Test Guideline A.14 of EC Directive 92/69/EEC.	-	1	Mak WA, 2004. [redacted]	X16

Section A3 Physical and Chemical Properties of Active Substance

				Conclusion: Considering the molecular structure and the information that is available in the literature, disodium octaborate tetrahydrate is not expected to have explosive properties in the sense of EC Directive 92/69/EEC.				
3.16	**Oxidizing properties (IIA3.12)**	-	-	-	In principle, inorganic substances that contain oxygen may show oxidizing properties and these should therefore be tested according to Test Guideline A.17 of EC Directive 92/69/EEC. However, a search of available literature has not resulted in any indication of oxidizing properties, neither has it shown any accident data that may be attributed to oxidizing properties. Conclusion: Considering the molecular structure and the information that is available in the literature, disodium octaborate tetrahydrate is not expected to have oxidizing properties in the sense of EC Directive 92/69/EEC.	-	1	Mak WA, 2004, [redacted]	X17
3.17	**Reactivity towards container material (IIA3.13)**	Suitable container materials: Paper, Cardboard, Plastic (Polypropylene, High density polyethylene) Unsuitable container materials: Base metals						

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.1.1. Melting point a. Three studies were summarized by the notifier without indication which study was considered as key study. Study 1 (Mellor's Comprehensive) is an encyclopedia and is given reliability 4 because no methods are described. Study 2 is a statement without references to analytical methods or purity of the active substance and is given reliability 4. Study 3 (Cordia et al., 2003) is considered as key study by the RMS because this study was carried out under GLP according to EC method A1 (= ASTM E 537-1) and with known purity. b. Although GLP was indicated for the key study, the report submitted, did not contain any authorisation signatures. An authorised report is not required as there is no hard GLP requirement. c. Experiments were carried out with batch number 225-01-444 [redacted] The purity of the active substance is given as 98%. The purity of the active substance in the key study (98%) complies with the minimum purity for the Borax Europe Ltd product (97.5%) but differs from the minimum purity indicated in chapter IIIA2.7 for the Societa Larderello spa product (99.7%). Data on impurities are not available. d. In the conclusion of the notifier pentaborate should be octaborate. e. The reference is stated wrong in the table. The full reference for the key study should be stated as: [redacted]
Conclusion	The melting point is 813/803 °C. A phase transition is found at 567 °C.
Reliability	study 1 and study 2 is reliability 4; study 3 is reliability 1 (key study)
Acceptability	acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	28-Apr-05
Materials and methods	Section 3.1.2. Boiling point. a. The notifier gives a statement that a boiling point is not applicable. The statement gives however phase transition points and boiling point values that are not confirmed by experiments. The reliability is set at 4. b. That a boiling point is not applicable, can be deduced from the melting point study (section A3.1.1) where no melting point was found in the range 25-1000 °C. A phase transition was found at 567 °C and a weak melting point was found at 813/803 °C. Therefore additional data are not required.
Conclusion	A boiling point is not applicable because the melting point lies above 360 °C. A phase transition was found at 567 °C and a melting point is found at 813/803 °C.
Reliability	study set at reliability 4.
Acceptability	acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.1.3. Relative density. a. Two studies were summarized by the notifier without indication which study was considered as key study. Study 1 is a technical data sheet without any indications on methods and is given reliability 4. Study 2 (Cordia et al., 2003) is considered as key study by the RMS because this study was carried out under GLP according to EC method EC method A3 (pycnometer method) and with known purity. b. Typing error: “a multi-volume pyncnometer” should be “a multi-volume pycnometer” c. Although GLP was indicated for the key study, the report submitted, did not contain any authorisation signatures. An authorised report is however not required as there is no hard GLP requirement. d. Experiments were carried out with batch number 225-01-444 ([redacted] The purity of the active substance is given as 98%. The purity of the active substance in the key study (98%) complies with the minimum purity for the Borax Europe Ltd product (97.5%) but differs from the minimum purity indicated in chapter IIIA2.7 for the Societa Larderello spa product (99.7%). Data on impurities are not available. e. The physical state of the measured substance is a solid. f. The relative density to water at 4 °C was calculated by dividing the absolute density with 1000.00 kg/m^3. The relative density is expressed as D^{22}_4, whereas it should be expressed as D^{20}_4. According to the notifier for solids the D^{22}_4 is equal to the D^{20}_4 within the experimental error. This is considered acceptable by the RMS. g. The reference is stated wrong in the table. The full reference for the key study should be stated as [redacted]
Conclusion	as indicated by the notifier for study 2
Reliability	study 1 reliability 4, study 2 reliability 1 (key study)
Acceptability	acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.2. Vapour pressure. a. The notifier submitted one study (Howarth et al., 1995) which is given reliability of 2 because the purity of the active substance is not indicated. b. Experiments were carried out with lot number 5B17[redacted]. Data on the purity of the active substance and data on impurities are not available. c. Vapour pressure was measured using EEC method A4 (effusion method, vapour pressure balance) which is suitable for the range 10^{-3} to 1 Pa. The vapour pressure indicated (9.9×10^{-17} Pa) lies outside this range. Therefore the RMS considers the value as not reliable. Although the gas saturation method or the spinning rotor method would have been preferred instead (suitable in the range 10^{-4} to 0.5-1 Pa), there are no methods to measure vapour pressures below 10^{-4} Pa. d. Temperature readings were taken in nine runs at temperatures between 41-250 °C. These temperatures lie all below the first phase transition point of 567 °C, where amorphous sodium borate is converted into crystalline sodium borate. Five of the nine balance readings could not be used because degassing was taking place. The remaining four balance readings at temperatures between 190-250 °C were extrapolated to 25 °C. Measurements in the key study indicate that the vapour pressure is less than 10^{-5} Pa. e. The full reference for the key study should be stated as: [redacted]
Conclusion	Not applicable, because the melting point lies above 300 °C and experimental data indicate that the vapour pressure at ambient temperature is less than 10^{-5} Pa.
Reliability	as indicated by the notifier.
Acceptability	acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	29-Apr-05
Materials and methods	Section 3.1.1, Henry's law constant The Henry's law constant can only be derived from the vapour pressure in combination with the aqueous solubility. Because the vapour pressure for disodium octaborate tetrahydrate is expected to be less than 10^{-5} Pa, no additional data are required.
Conclusion	Not applicable. At ambient temperature, vapour pressure is expected to be less than 10^{-5} Pa.
Reliability	-
Acceptability	acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.3 Appearance Physical state, color and odour is stated without specification of the purity of the active substance, impurities present, temperature and pressure.
Conclusion	as indicated by the notifier
Reliability	as indicated by the notifier.
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.4 Spectra a. Two studies were submitted. Study 1 contains data and is considered as key study by the RMS because GLP is indicated and data were obtained according to guidelines. Study 2 is a statement on NMR and is given reliability of 4. b. Although GLP was indicated for the key study, the report submitted, did not contain any authorisation signatures. An authorised report is however not required as there is no hard GLP requirement. c. Experiments were carried out with batch number 225-01-444 [redacted] The purity of the active substance is given as 98%. The purity of the active substance in the key study (98%) complies with the minimum purity for the Borax Europe Ltd product (97.5%) but differs from the minimum purity indicated in chapter IIIA2.7 for the Societa Larderello spa product (99.7%). Data on impurities are not available. d. UV/VIS spectra were recorded between 190-500 nm. According to OECD 101 guideline, the spectrum should be recorded between 200-750 nm. The recording was stopped too early. But for a salt like sodium octaborate tetrahydrate without absorption in the area between 190-500 nm, an absorption in the area between 500-750 nm is not to be expected. e. FTIR spectra were recorded between 400-4000 cm^{-1}. Peaks were observed at 696 (narrow), 785 (narrow), 1047 (broad), 1339 (broad), 3435 (broad) cm^{-1}. f. In study 2, a statement was given that ^{13}C-NMR spectra are not applicable, because disodium octaborate tetrahydrate does not contain carbon atoms. The study is given reliability of 4. Although ^{11}B-NMR or ^{17}O-NMR are more appropriate, these instruments are not available in most laboratories. g. MS data could not be obtained when an instrument designed for organic substances was used (liquid chromatography - flow injection- electrospray mass spectrometry with Q-TOF). h. Another technique which is appropriate to elucidate the structure of disodium octaborate is Raman spectroscopy or X-ray spectroscopy. Spectral data for these techniques are welcome. i. The reference is stated wrong in the table. The full reference for the key study should be stated as: [redacted] j. The full reference for the NMR statement study should be stated as: [redacted]

Conclusion	No absorption maximum or minimum was found in the UV/VIS spectrum in neutral, basic or acidic medium in the range 190-500 nm and no absorption is expected in the range 500-750 nm. FTIR spectra of disodium octaborate tetrahydrate recorded as KBr pellet revealed peaks at 696 (narrow), 785 (narrow), 1047 (broad), 1339 (broad), 3435 (broad) cm^{-1}. ^{13}C-NMR spectra are not applicable, because disodium octaborate tetrahydrate does not contain carbon atoms. MS spectra could not be obtained because solutions of disodium octaborate tetrahydrate could not be ionised in a HPLC-ES-MS system.
Reliability	key study set at 1; NMR statement set at 4.
Acceptability	acceptable.
Remarks	Raman spectroscopy and X-ray spectroscopy data are desirable.
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.5 Water solubility. a. The water solubility for disodium octaborate tetrahydrate as such cannot be determined because disodium octaborate tetrahydrate is converted into boric acid/borate upon dissolution in water: $Na_2B_8O_{13}.4H_2O + 9H_2O \leftrightarrow 2NaB(OH)_4 + 6\ B(OH)_3$. The water solubility found will be the water solubility for boric acid in the presence of sodium ions. b. Two studies were summarized by the notifier without indication which study was considered as key study. Study 1 (Kirk-Othmer) is an encyclopedia without description of methods or purity of the active substance. Study 1 is set at reliablity 4 and is used as confirmation study. Study 2 (Cordia et al., 2003) is considered as key study by the RMS because this study was carried out under GLP according to EC method A6 (flask method) and with known purity. c. Although GLP was indicated for the key study, the report submitted, did not contain any authorisation signatures. An authorised report is however not required as there is no hard GLP requirement. d. Experiments were carried out with batch number 225-01-444 [redacted] The purity of the active substance is given as 98%. The purity of the active substance in the key study (98%) complies with the minimum purity for the Borax Europe Ltd product (97.5%) but differs from the minimum purity indicated in chapter IIIA2.7 for the Societa Larderello spa product (99.7%). Data on impurities are not available. e. The solubility was determined by EC method A6 (flask method) and samples were analysed by HPLC with refractive index detection. The notifier indicates that this method produces a supersaturated solution and proposes to determine the solubility by precipitation from an oversaturated solution and measuring the solubility of the remaining solution. This experiment was not carried out, but is recommended to confirm the value given in literature. f. The key study determines the water solubility by dissolving the substance in water (resulting pH=7.64), whereas the effect of pH (5 to 9) must be studied. Water solubility studies at pH=5, 7, 9 are not possible, because of the strong buffering capacity of boric acid/borate solutions and ion-pair formation in the presence of alkali-metal ions like Na, K. No further data are required. g. In the Kirk-Othmer encyclopedia (study 1) a temperature dependence of water solubility is indicated. However, since water solubility is very high, a study on temperature dependence is unlikely to yield relevant data for the risk assessment. h. The reference is stated wrong in the table. The full reference for the key study should be stated as: [redacted]

Conclusion	The water solubility for disodium octaborate tetrahydrate as such cannot be determined because disodium octaborate tetrahydrate is converted into boric acid/borate upon dissolution in water: $Na_2B_8O_{13}.4H_2O + 9H_2O \leftrightarrow 2NaB(OH)_4 + 6\ B(OH)_3$. The water solubility found will be the water solubility for boric acid in the presence of sodium ions. The water solubility of disodium octaborate tetrahydrate is 223.65 ± 6.73 g/L at 20 °C (super saturated solution), resulting in a pH of 7.64. Water solubility studies at pH=5, 7, 9 are not possible, because of the strong buffering capacity of boric acid/borate solutions and ion-pair formation in the presence of alkali-metal ions like Na, K.
Reliability	study 1 (Kirk-Othmer), set at 4. study 2 (Cordia et al., 2003), set at 1 (key study)
Acceptability	Acceptable.
Remarks	-

	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	26-Jan-05
Materials and methods	Section 3.6 Dissociation constant. a. The notifier indicates that a dissociation constant is not required but without any statement why. A dissociation constant is required because the active substance has weak basic properties (pH = 7.64 for a supersaturated solution and pH=8.5 for a saturated solution). b. The dissociation constant for disodium octaborate tetrahydrate as such cannot be determined because disodium octaborate tetrahydrate is converted into boric acid/borate upon dissolution in water: $Na_2B_8O_{13}.4H_2O + 9H_2O \leftrightarrow 2NaB(OH)_4 + 6\ B(OH)_3$. The dissociation constant found will be the dissociation constant for boric acid in the presence of sodium ions. Therefore, information on boric acid is copied into the present document. c. For the determination of the dissociation constant, five studies were submitted by the notifier without indication which study was considered as key study. None of the studies is considered reliable enough to be a key study by the RMS. Two of the studies submitted were not summarized by the notifier: Hahn and Klockman, 1930 and Kankaanpera and Salomaa, 1969. Hahn and Klockman, 1930, and Jenkins, 1945 give a theoretical calculation model for the dissociation constant of boric acid and metaboric acid (HBO_2) respectively. Calculated values for these compounds are not reported and experimental values are not available. The reliability is set at 4. Bell et al, 1967 and Kankaanpera and Salomaa, 1969 review on the structure of the borate ions. The structures found with Raman spectrometry and NMR were the uncharged $B(OH)_3$ and $[B(OH)_4]^-$. Boron concentration was however not indicated. The dissociation constant for this equilibrium was reported as pKa=9.2. Methods were however not indicated and the reliability is set at 4 for both studies. WHO, 1998 reports a pKa= 9.15 in dilute aqueous solutions of boric acid. Methods were however not indicated and the reliability is set at 4. Although the notifier indicates a purity of 99.0 to 100.5%, no purity indications are given in the study reports cited above. --- In study report, De Vette, 2001, Raman spectroscopy was used to identify species in 0.02 M boron solutions of boric acid, disodium tetraborate decahydrate and disodium octaborate tetrahydrate in non-buffered and buffered solutions at pH 6.0, 7.0, 8.0 and 9.0. In all solutions prominent peaks for undissociated $B(OH)_3$ were found. Depending on pH also peaks for $B(OH)_4^-$ and polyborate anions were found. d. The references from document IIIA6.2-A10 read across for disodium octaborate tetrahydrate contained additional information on dissociation constants: Ingri, 1963 investigated the behaviour of boric acid at different pH values and different ion strengths at 25 °C using potentiometric titration with hydrogen or glass electrodes. The author concluded that in acid solution at pH<5, boron is mainly present at $B(OH)_3$ and in alkaline solution at pH>12.5, boron is mainly present as $B(OH)_4^-$.

At intermediate pH-values, for B ≤ 0.025 M, a mixture of $B(OH)_3$ and $B(OH)_4^-$ was found and for B > 0.025 M also polynuclear complexes were found. In an inert medium of 3 M $Na(ClO_4$, OH) or 3M Na(Br) or 3M Li(Br), polynuclear $B_3O_3(OH)_4^-$ was found and both $B_3O_3(OH)_5^{2-}$ and $B_4O_5(OH)_4^{2-}$. When the medium was changed into 3 M K(Br) the $B_3O_3(OH)_5^{2-}$ complex was not formed. In a self-medium of 3 M $Na(B(OH)_4$, OH) at alkaline pH-values the polynuclear $B_4O_5(OH)_4^2$ was found in addition to small amounts of $B_3O_3(OH)_5^{2-}$. In an inert medium of 0.1 or 3 M $Na(ClO_4$, OH) and at high boron concentrations mainly $B_5O_6(OH)_4^-$ was found.

Therefore, at pH-values between 5-12, an equilibrium is formed between $B(OH)_3$, polynuclear complexes of $B_3O_3(OH)_4^-$, $B_4O_5(OH)_4^{2-}$, $B_3O_3(OH)_5^{2-}$, $B_5O_6(OH)_4^-$ and $B(OH)_4^-$. In short: $B(OH)_3$ ↔ polynuclear anions ↔ $B(OH)_4^-$. At low boron concentrations (B ≤ 0.025 M) the equilibrium changes into $B(OH)_3$ ↔ $B(OH)_4^-$. For the latter equilibrium a pK_a value of 9.00 ± 0.05 was obtained at 25 °C. At higher boron concentrations the other species must be taken into account. Ingri, 1963 determined equilibrium constants for each of the species. The disscociation constants for the polynuclear anions require complex formulas and are considered not relevant for the present evaluation.
The reliability is set at 2 for this study.

In Maeda, 1979, Raman spectra were taken from 1.5 M boron solutions with pH values of 6.4 - 7.4 - 8.3 - 9.4 obtained by mixing appropriate amounts of boric acid and sodium hydroxide. At all pH values, both $B(OH)_3$ and $B(OH)_4^-$ were present as well as three different polyborate ions: $B_5O_6(OH)_4^-$, $B_3O_3(OH)_4^-$, $B_4O_5(OH)_4^{2-}$.

In Farmer, 1982, an overview is given on borate dissociation studies. Because no methods are indicated, the reliability is set at 4. The study can only be used as background information.
Based on NMR data, the reactions can be described as the interaction of boric acid with the borate anion:

a. $B(OH)_3 + 2H_2O \leftrightarrow [B(OH)_4]^- + H_3O^+$ pKa1 = 9.0

b. $4B(OH)_3 + [B(OH)_4]^- \leftrightarrow [B_5O_6(OH)_4]^- + 6H_2O$ pKa5 = 6.8

c. $2B(OH)_3 + [B(OH)_4]^- \leftrightarrow [B_3O_3(OH)_4]^- + 3H_2O$ pKa2 = 6.8

d. $2B(OH)_3 + 2[B(OH)_4]^- \leftrightarrow [B_4O_5(OH)_4]^{2-} + 5H_2O$ pKa4 = 14.8

e. $B(OH)_3 + 2[B(OH)_4]^- \leftrightarrow [B_3O_3(OH)_5]^{2-} + 3H_2O$ pKa3 = 16.5

Borate equilibrium constants are influenced by group I metal salts (Na, K, Cs) and temperature. In the presence of NaCl, Ka1 becomes larger and Ka4 smaller as temperatures increase. With increasing size of hydrated cation (Na, K, Cs) Ka1, Ka2 and Ka4 increase. Maximum values of Ka1, Ka2, Ka3, Ka4 are reached in saturated salt solutions.

Raman spectroscopy confirmed the structures in aqueous solutions. At pH=4.2 only boric acid was found. At pH=11 $B(OH)_4^-$ was found and a slight amount of polyanions (unresolved broad band). At pH=8.3 boric acid, $B(OH)_4^-$ as well as polyanions $[B_3O_3(OH)_4]^-$, $[B_4O_5(OH)_4]^{2-}$, $[B_5O_6(OH)_4]^-$ and $[B_3O_3(OH)_4]^-$ were found. No evidence of $B_3O_3(OH)_5]^{2-}$ was found.

In the presence of metal ions (e.g. Na, Mg, Sr, Ba, Ca, Fe) ion-pair complexes are formed, which further reduce the undissociated boric acid concentration. For the equilibrium $M^{n+} + B(OH)_4^- \leftrightarrow MB(OH)_4^{(n-1)+}$ logarithmic dissociation constants of -1.63, -1.80, -1.56, -1.50 and -0.22 were found for M= Mg, Ca, Sr, Ba and Na.

In Encyclopedia, Kirk-Othmer, 1992, the equilibrium constant for dilute solutions of boric acid (<0.1 M) for the equilibrium of $B(OH)_3 + 2\,H_2O \leftrightarrow [B(OH)_4]^- + H_3O^+$ is reported to be 5.8×10^{-10} at 25 °C. This corresponds to a pKa value of

9.24. Calculated pH values based on this constant deviate considerably from measured ones as the boric acid concentration is increased, as is shown in the table. Methods were however not indicated and the reliability is set at 4.

B(OH)3 conc	pH observed	pH calculated
0.0603 M	5.23	5.23
0.0904 M	5.14	5.14
0.1205 M	5.01	5.08
0.211 M	4.71	4.96
0.422 M	4.22	4.80
0.512 M	4.06	4.76
0.753 M	3.69	4.54

In textbook, Holleman, 1995, the dissociation constant is reported as pKa = 9.25 for a diluted solution of boric acid. Methods were however not indicated and the reliability is set at 4.

References

Ingri N. Equilibrium studies of polyanions containing B^{III}, Si^{IV}, Ge^{IV} and V^{V}. Sven. Kem. Tidskr. 1963;75(4):199-230.

Maeda M, Raman Spectra of polyborate ions in aqueous solution. J Inorg. Nucl. Chem., Vol 41, pp 1217-1220 (1979)

Farmer, 1982 Structural Chemistry in the Borate Industry., Chem and Ind.,

Kirk – Othmer Encyclopedia of Chemical Technology, V4, 1992, pp 378-380

Holleman, 1995. Lehrbuch der anorganischen Chemie. 101st ed de Gruyter, Berlin, copyright

De Vette, [redacted], 2001 Hydrolysis as a function of pH and identification of breakdown products. [redacted]

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d. None of the studies was carried out according to OECD 112. The study of Ingri, 1963 is considered as key study and together with the other studies a good overview is obtained about processes occurring when boric acid is dissolved in water.

Conclusion

The dissociation constant for disodium octaborate tetrahydrate as such cannot be determined because disodium octaborate tetrahydrate is converted into boric acid/borate upon dissolution in water: $Na_2B_8O_{13}.4H_2O + 9H_2O \leftrightarrow 2NaB(OH)_4 + 6\ B(OH)_3$. The dissociation constant found will be the dissociation constant for boric acid in the presence of sodium ions.

At low boron concentrations (B ≤ 0.025 M) the following equilibrium is found

$B(OH)_3 + 2H_2O \leftrightarrow [B(OH)_4]^- + H_3O^+$ pKa = 9.0 at 25 °C

In dilute aqueous solutions (B ≤ 0.025 M) boric acid exists as undissociated boric acid $B(OH)_3$ at pH < 7, at pH > 11 the metaborate ion $[B(OH)_4]^-$ becomes the main species in solution. At inbetween values (pH 7-11) both species are present.

At higher boron concentrations (B > 0.025 M) an equilibrium is formed between $B(OH)_3$, polynuclear complexes of $B_3O_3(OH)_4^-$, $B_4O_5(OH)_4^{2-}$, $B_3O_3(OH)_5^{2-}$, $B_5O_6(OH)_4^-$ and $B(OH)_4^-$. In short: $B(OH)_3 \leftrightarrow$ polynuclear anions $\leftrightarrow B(OH)_4^-$.

	In acid solution at pH<5, boron is mainly present at $B(OH)_3$ and in alkaline solution at pH>12.5, boron is mainly present as $B(OH)_4^-$. At inbetween values (pH 5-12) polynuclear anions are found as well as $B(OH)_3$ and $B(OH)_4^-$. The dissociation constant depends upon temperature, ionic strength and presence of group I metal ions (Na, K, Cs). In the presence of metal ions (e.g. Na, Mg, Ca) ion-pair complexes are formed, which further reduce the undissociated boric acid concentration: $M^{n+} + B(OH)_4^- \leftrightarrow MB(OH)_4^{(n-1)+}$ These ion pair complexes are expected to be present in solutions of disodium tetraborate, disodium octaborate and buffered solutions of boric acid and boric oxide.
Reliability	-
Acceptability	acceptable
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	26-Jan-05
Materials and methods	Section 3.7 Solubility in organic solvents. Solubility in organic solvents is not considered required as results will not be relevant for the risk assessment of the a.s.. Critical endpoints, like the log Pow that depend on the solubility in organic solvents were experiementally determined.
Conclusion	No data available; not required
Reliability	-
Acceptability	Acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	26-Jan-05
Materials and methods	Section 3.8 Stability in organic solvents Data are not required because the active substance does not contain any organic solvents.
Conclusion	Data are not required because the active substance does not contain any organic solvents.
Reliability	as indicated by the notifier.
Acceptability	acceptable.
Remarks	-
	COMMENTS FROM ...
Date	*Give date of comments submitted*
Results and discussion	*Discuss additional relevant discrepancies referring to the (sub)heading numbers and to applicant's summary and conclusion.* *Discuss if deviating from view of rapporteur member state*
Conclusion	*Discuss if deviating from view of rapporteur member state*
Reliability	*Discuss if deviating from view of rapporteur member state*
Acceptability	*Discuss if deviating from view of rapporteur member state*
Remarks	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	16-Sept-05
Materials and methods	Section 3.9 Partition coefficient. a. The notifier submitted one study (Barres, 1967) . The study concerns the partition coefficient for boric acid and borates and is considered relevant for the present evaluation (reliability set at 2). b. The notifier submitted a statement that the partition coefficient for disodium octaborate tetrahydrate cannot be measured because the substance breaks down to boric acid and disodium tetraborate. The RMS agrees that the partition coefficient for disodium octaborate tetrahydrate as such cannot be determined because disodium octaborate tetrahydrate is converted into boric acid/borate upon dissolution in water: $Na_2B_8O_{13}.4H_2O + 9H_2O \leftrightarrow 2\ NaB(OH)_4 + 6\ B(OH)_3$. The partition coefficient found will be the partition coefficient for boric acid in the presence of sodium ions. Therefore, information on boric acid is copied into the present document. c. Two studies on boric acid were summarized by the notifier without indication which study was considered as key study. Study 2 (Cordia et al., 2003) is considered as key study by the RMS because this study was carried out under GLP according to EC method A8 and with known purity. Study 1 (Barres, 1967) is given reliablity 2 because the study was not carried out under GLP. d. Although GLP was indicated for the key study, the report submitted, did not contain any authorisation signatures. An authorised report is however not required as there is no hard GLP requirement. e. The key study was carried out with batch number 225-01-442 [redacted]. The purity of the active substance is given as 99.0-100.5%. Data on impurities are not available. f. The key study was carried out with the shake flask method. Concentrations in the samples were determined by HPLC with refractive index detection. Boric acid was dissolved in a potassium/sodium phosphate buffer pH=7.5 at 22 °C at a concentration of 0.5972 g/L (0.00966 M boron). At concentrations below 0.025 M boron an equilibrium is formed between $B(OH)_3$ and $B(OH)_4^-$. The estimated pK_a value for this equilibrium is 9.0 (see IIIA3.7) and at pH=7.5 boric acid will be present at approximately 97% in the non-ionized form $B(OH)_3$ and for 3% in the ionized form. Possibly the $B(OH)_3$ concentration is reduced because of ion pair formation between potassium or sodium and the $B(OH)_4^-$ ions. g. The alternate study (Barres, 1967) was carried out with the shake flask method. Concentrations in the samples were determined by electrometry. Boric acid, analytical grade, was recrystallized to unknown purity. Boric acid was dissolved in decarbonated water without buffer system at 25 °C at various concentrations. Upon equilibrium concentrations in the aqueous phase varied between 0.16 - 0.89 M boron. At boron concentrations above 0.025 M, an equilibrium is formed between $B(OH)_3$, $B(OH)_4^-$ and polyborate anions. The resulting pH value was not measured. The log Pow value found (-0.757 ± 0.004) was independent of boric acid concentration. The partition coefficient value of -0.757 from this study was used in the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh).