Document III-A: Study Summaries - Active Substance, Boric Oxide

Section A1 Applicant

Annex Point IIA1

Official use only

1.1 Applicant

Contact: [redacted]
2 Eastbourne Terrace
London, W2 6LG
United Kingdom
[redacted]
Website: www.riotinto.com

X1

1.2 Manufacturer of Active Substance (if different)

Boric Oxide imported by Rio Tinto Minerals is manufactured in the USA

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

X2

	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-June-08
Materials and methods	Section 1.1 Applicant The first applicant/notifier name is Lead Notifier: Rio Tinto Minerals (see boric acid section IIIA1). The whole address is changed.
Conclusion	**Lead notifier: Rio Tinto Minerals** Contact: [redacted] *2 Eastbourne Terrace* *London, W2 6LG* United Kingdom [redacted] *Website:* www.riotinto.com
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	14-Sept-05
Materials and methods	Section 1.2 Manufacturer For US Borax Inc the whole address is changed.
Conclusion	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, Boric Oxide

Section A2 Identity of Active Substance

Subsection (Annex Point)			Official use only
2.1	**Common name (IIA2.1)**	Boric Oxide; Anhydrous Boric Acid boron trioxide; diboron trioxide; boric anhydride; anhydrous boric acid	X1
2.2	**Chemical name (IIA2.2)**	diboron trioxide	
2.3	**Manufacturer's development code number(s) (IIA2.3)**	Not relevant	
2.4	**CAS No and EC numbers (IIA2.4)**		X2
2.4.1	**CAS-No**	1303-86-2	
2.4.2	**EC-No**	215-125-8	
2.4.3	**Other**		
2.5	**Molecular and structural formula, molecular mass (IIA2.5)**		
2.5.1	**Molecular formula**	B_2O_3	
2.5.2	**Structural formula**	The solid state boric oxide consists of boroxyl rings and probably is an infinite polymeric structure. See structure attached to IUCLID database	X3
2.5.3	**Molecular mass**	69.82	X4
2.6	**Method of manufacture of the active substance (IIA2.1)**	[redacted] [redacted] [redacted] [redacted] [redacted] [redacted] [redacted] [redacted]	X5

Section A2 Identity of Active Substance

[redacted]

[redacted]

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

Boric Oxide	% w/w	
	B2O3	**Purity**
Typical	98.4	98.4
Maximum	100.0	100.0
Minimum	97.5	97.5

X6

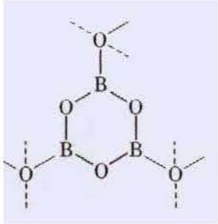
2.9 The origin of the natural active substance or the precursor(s) of the active substance (IIA2.9)

Natural inorganic mineral ore

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

	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 2.1: Common name a. common name should be discerned from synonyms and trade names b. other synonyms are boron oxide (CRC Handbook of Chemistry and Physics, 1999) and boron sesquioxide (Merck Index on CD-rom, version 12.1, 1996).
Conclusion	Common name: boric oxide Synonyms: synonyms: boron oxide, boron sesquioxide, boron trioxide, diboron trioxide, boric anhydride, anhydrous boric acid. Trade names: not available
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	15-Sept-05
Materials and methods	Section 2.4 CAS number and EC number a. In the 29th ATP, 27th May 2003 the following decisions were made: Boric oxide or diboron trioxide, CASno 1303-86-2, EC no 215-125-8. These numbers correspond with the numbers submitted by the notifier. b. On the ECB website, two CAS numbers and two EC numbers exist. * Boric oxide, CASno 1303-86-2, EC no 215-125-8 * Boric oxide, unstated purity, CAS no 54566-73-3, EC 259-231-2. For this CA-report, CAS no 1303-86-2 is used (pure boric oxide). CAS no 54566-73-3 has an unstated purity and is not assessed in this CA-report.
Conclusion	Two CAS numbers exist for the same compound. * Boric oxide, CASno 1303-86-2 * Boric oxide, unstated purity, CAS no 54566-73-3. For this CA-report, CAS no 1303-86-2 is used (pure boric oxide). CAS no 54566-73-3 has an unstated purity and is not assessed in this CA-report. Two EC numbers exist for the same compound. * Boric oxide, EC no 215-125-8. * Boric oxide, unstated purity, EC no 259-231-2. For this CA-report, EC no is 215-125-8 is used (pure boric oxide). EC no 259-231-2 has an unstated purity and is not assessed in this CA-report.
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 2.1: Structural formula The notifier refers to the IUCLID database for the structural formula. The structural formula should also be given here.
Conclusion	Structural formula: 
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 2.5.3: Molecular mass It is not clear where the molecular mass as submitted by the notifier came from. The molecular mass is given as 69.62 in the CRC Handbook of Chemistry and Physics, version 1999. This molecular mass is used throughout the CA-report.
Conclusion	Molecular mass is 69.62
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 The manufacturing process for Borax Europe Limited is considered as an industrial scale process, although this is not indicated by the notifier.
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	28-Apr-05
Materials and methods	Section 2.7: Purity of the active substance a. The specification data cannot be verified by the RMS, because batch analyses are not submitted. These are however not required. b. The specification data as indicated here comply with the impurity data and the data for the compounds used in the tests for physical chemical properties. c. The table gives information on B2O3 purity and purity, which is twice the same compound and twice the same value. One column can be deleted.
Conclusion	Based on impurity data and tests with the active substance, the minimum purity specification of 97.5% for the active substance is realistic. Maximum purity is 100%.
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, Boric Oxide

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

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

Subsection (Annex Point)		**Official use only**
2.8 Identity of impurities and additives, as appropriate (IIA2.8)	Major impurities measured in Boric oxide manufactured in the USA by US Borax and sold by Borax Europe for Biocidal Use:	X1

Boric Oxide	**% w/w**	
	Fe	**SO_4**
Typical	0.0005	0.0070
Maximum	0.0010	0.0250
Minimum	0.0000	0.0000

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%.

2.8.1 Isomeric composition	Not relevant				
2.8.1.1 Common name	Not relevant				
2.8.1.2 Function					
2.8.2 IUPAC name					
2.8.3 CAS-No					
2.8.4 EC-No					
2.8.5 Other					
2.8.6 Molecular formula					
2.8.8 Molecular mass					
2.8.9 Concentration of the impurity or additive *typical and range of concentrations*		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, sulphate
RMS 2.8.1.1. Function	impurity of starting material
RMS 2.8.2 IUPAC name	not applicable
RMS 2.8.3 CAS no	not applicable
RMS 2.8.4 EC no	not applicable
RMS 2.8.5 Other	not applicable
RMS 2.8.6 Molecular formula	Fe, SO_4
RMS 2.8.7 Structural formula	unknown
RMS 2.8.8 Molecular mass	Fe = 55.845 SO_4 = 32.066(6) + 4x 15.9994(3) = 96.043 Reference: CRC Handbook of Chemistry and Physics, 1999
RMS 2.8.9 Concentration of impurity or additive *typical and range of concentrations*	Major impurities measured in Boric oxide manufactured in the USA by US Borax and sold by Borax Europe for Biocidal Use:

Boric Oxide	% w/w	
	Fe	SO_4
Typical	0.0005	0.0070
Maximum	0.0010	0.0250
Minimum	0.0000	0.0000

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%.

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	1 EVALUATION BY RAPPORTEUR MEMBER STATE
Date	15-Sept-05
Materials and methods	Section 2.8 Impurities a. The summary written by the notifier is not according to template. Therefore the whole section was rewritten by the RMS. b. The specification data for impurities cannot be verified by the RMS, because batch analyses are not submitted. These are, however, not required. c. The specified impurities for the boric oxide product add up to a maximum of 0.0251% w/w and this level complies with the minimum purity requirement of 97.5% (w/w) for boric oxide.
Conclusion	Maximum specified impurities are compliable with the minimum purity of 97.5% (w/w) expressed as B_2O_3.
Reliability	-
Acceptability	acceptable
Remarks	-
	2 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, Boric Oxide

Section A2.10 — 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

Annex Point IIA2.10

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)

1. Professional /Industrial Users

i) Description of application process	Boron rods are supplied ready prepared and are inserted in predrilled holes that are later sealed. Sealing the rods creates a hydrophobic barrier that limits water and boron movement out of the pole. In addition for Hazard Class 3 and 4a the treated areas is sealed with a water resistant coating (an exterior grade wood coating) to prevent leaching out of the active ingredient.
ii) Workplace description	In buildings or outside
iii) Inhalation exposure	Clear cylindrical fused glass rod and boric oxide is non volatile, therefore there is no inhalation exposure
iv) Dermal exposure	The dermal exposure and risks from using such rods is so small as to be minimal and can be excluded as described in the Technical Notes for Guidance- Human Exposure to Biocidal Products (TNG; EC 2002) and Technical Guidance Document on Risk Assessment (TGD; ECB 2003 page 46(and 47) in Section 3.v.3 of "Assessment of Human Exposures to Biocides" (Report to DG XI From the Biocides Steering Group, October 1998), where indeed, a portion of boric oxide rod scenario is used as an example of an insignificant exposure scenario that need not be quantitatively evaluated "...where the foreseeable exposure is so low as to be able to dismiss the risk, e.g., inserting solid borate rods in pre-drilled holes" (ECB, 2003).

2. Non-professional Users including the general public

Boron rods are available for the Amateur market and like the Professional users above the exposures are insignificant and can be excluded. No specific protective clothing can be assumed (i.e. no gloves worn). However, to confirm this there several points can be made

1. The Rods are non irritant, therefore no protection is needed

2. The dermal absorption of borates is < 0.4% with a flux of 0.009 µg/cm^2 /h and varies little among the 3 borates tested therefore the dermal absorption of boric oxide can be assumed to be consisted with that of boric acid. The average surface area of a hand is 410 cm^2. Over a 5 hour period at a flux of 0.009 µg/cm^2 /h, only 18.5µg of boric oxide would be absorbed. This is equivalent to 5.7 µg of boron or 0.08µg B/kg (70 kg weight) and provides an MOE of 1.2 x10^{5}over the NOAEL of 9.6 mg B/kg/day that is negligible.

Therefore there is no risk to human health associated with handling boron rods with or without hand protection.

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

2.10.2.2 Intended use(s)

Products to be protected:

Timbers exposed to risk of attack by wood destroying organisms. For example:

Use Class 1 timbers under cover including indoor joinery (preventive)

Use Class 2 timbers under cover including indoor roofing timbers – risk of wetting (preventive)

Use Class 3 exterior timbers out of ground contact including joinery protected with a surface coating (preventive)

Use Class 4a remedial application to timbers in service in ground contact e.g. boron rods inserted into utility poles which are already in service and may have been treated in the past with creosote (curative and preventive).

For Hazard Classes 1 &2 emissions are not expected as indicated in OECD Series on Emission Scenario Documents No 2 for Wood Preservatives Part 1 (2002*)*

For Hazard Class 3, treatment with a water resistant coating (an exterior grade wood coating) to create a hydrophobic barrier that limits water movement and therefore emissions will not be expected.

Affected compartment(s):

For Hazard Class 3b and 4a – minimal leaching occurs and studies have shown that 60% of the boron from rods in exposed, sealed wood is still present in the wood after 6 years (McCormack and Dickinson, 1993).

Soil

The original boron content in a rod is approximately 2.5 grams, an average flux of 0.5 mg/day is calculated (Table 1) over 6 years. Results of cross-sectional analyses conducted by McCormack and Dickinson (1993) indicate that retention in the centre portions of the wood are much greater than retention near the surface of the wood. Therefore, this flux rate should be assumed to represent an overestimate of actual leaching over the lifetime of the treated wood. Assuming this flux rate is constant over an exposure period, it is calculated that it would take 15 years for all the boron to leach from a rod. It is unlikely that the flux rate would be constant over the entire 15-year period, but would likely drop over time as the boron in the outermost portions of the wood is selectively lost over time.

An estimation assuming of the boron leached throughout those 15 years that will remain in soil in an impacted area that has a 10 cm radius and is 50 cm deep (consistent with assumptions used in the EUSES model), is shown. However this assumes that all the boron has reached out after 15 years which is unlikely to occur.

Boron	**Boron Concentration in Soil**	
	6 years	15 Years
	1.85 mg B/kg	2.61 mg B/kg

Worldwide, B concentrations range from 10-300 mg kg^{-1} (average 30 mg kg^{-1}), depending on the type of soil, amount of organic matter, and amount of rainfall (IPCS, 1998)

Water

Surface Water Compartment. This analysis is parallel to the one conducted above for soil. The same leaching assumptions described above for soil were used, but instead of assuming that the leached boron stays in soil, it is assumed that all the boron leached from one rod over the entire 15-year period will reach a surface water body. Consistent with OECD emission scenarios, it is assumed that the receiving surface water body is flowing at a rate of 0.3 m^3/sec consistently over the entire 15-year period, a surface water concentration of $1.1x10^{-8}$ mg/L is estimated (.0097 nanograms B per liter; ng B/L). This is far below background water levels of Boron (Wyness et al., 2003)

References:

IPCS, 1998. Environmental Health Criteria 204: Boron. International Programme on Chemical Safety involving US EPA, UNEP, WHO and International Labour Organisation, CI, USA

.McCormack P.W. and D.J. Dickinson. 1993. Collaborative Project to Assessment the Effectiveness of Boron Rods as a Secondary Preservative Treatment in Wood Poles. Imperial College of Science Technology and Medicine. Final Report.

Wyness et al. 2003 A summary of boron surface water quality data throughout the European Union. Science of the Total Environment 2003: (314-316), 255-269

	Evaluation by Competent Authorities
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	4-Oct-05
Materials and methods	Section IIIA2.10 Human exposure assessment a. The application of boric oxide fused rods is described In Doc III A A2.10.1. It is stated that there is no inhalation exposure as boric oxide is not volatile, which is correct.Concerning the dermal exposure the notifier stated that the dermal exposure and risks can be excluded.No models were found which can describe the exposure due to the application of fused rods. Considering the application process the exposure will in any case be much smaller than the exposure during and after application of the other borates (boric acid, disodium tetraborates (anhydrous, pentahydrate, decahydrate), disodium octaborate decahydrate). Environmental exposure assessment b. 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 and following subsections.
Conclusion	Human exposure assessment In Doc IIB, section 8 ‘Exposure Assessment’ the calculations which we have done are reported. The exposure to boron is calculated for application of boric acid, disodium tetraborate decahydrate (borax) and disodium octaborate (DOT), the exposure due to boric oxide fused rods will be much smaller than the calculated values. 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 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	

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								X1
Melting pt. 1	No data	No data	**result:** 325-450°C	The value is for vitreous rather than crystalline boric oxide.	No data	2	Mellor's Comprehensive Treatise on Inorganic & Theoretical Chemistry, Volume V Boron, Part A: Boron-Oxygen Compunds, Longman London and New York, (1980), ISBN 0-582-46277-0, page 178.	
Melting pt. 2	ASTM E537-86, Method 102 of OECD Guidelines. (Differential Scanning Calorimetry).	97.5-100.0%	**result:** >360°C Temperature range: 25-360°C.	Endotherm observed at ~100°C which is interpreted as the loss of free water. Small endotherms observed between 140 and 160°C approx., which is interpreted as possible loss of water of crystallisation.	Y	1	Cuthbert J.E., [redacted] 2003, [redacted]	
3.1.2 Boiling point								X2
Boiling pt. 1	No data	No data	**result:** 2316°C (extrapolated) **pressure:** No data	Since boric oxide has a boiling point of 2200°C, a boiling point determination is not relevant. An estimate has been extrapolated from Kirk-Othmer, 1992.	No data	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons Inc., New York, 1992, 4th Edition, Volume 4, page 369.	

3.1.3 Bulk density/ relative density								X3
Bulk/rel. density 1	No data	No data	density = 1.84 g/cm^3 at 20°C.	The physical properties of boric oxide, particularly density, are somewhat dependant on moisture and thermal history. The value reported was determined on material with low water content.	No data	2	Mellor's Comprehensive Treatise on Inorganic and Theoretical Chemistry, Volume V Boron, Part A: Boron-Oxygen Compounds, Longman London and New York, (1980), ISBN 0-582-46277-0, page 174-176	
Bulk/rel. density 2	OECD Guidelines Method 109 (using a gas comparison pycnometer).	97.5-100.0%	density = 1.84 x 10^3 kg/m^3 at 21.5 ± 0.5°C.	The relative density was determined with vitreous boric oxide. (Refer to Document IIIA, Section 2.6, Manufacturing Process).	Y	1	Cuthbert J.E., [redacted] 2003.	
3.2 Vapour pressure (IIA3.2)								X4
Vapour pressure 1	Directive 92/69/EEC A.4	Boric acid 99.95%	**temperature:** 25°C **result:** 9.9×10^{-8} hPa	At ambient temperature the vapour pressure is negligible. The vapour pressure of boric oxide can be calculated from the following equation: logp = 5.849 – 16960/t over the temperature range 1331-1808°K. Many of the uses of boric oxide involve high temperatures e.g. glass manufacture. (Mellor, 1980). However, the vapour pressure of boric acid is very low and can be extrapolated to boric oxide, as boric oxide is hygroscopic and takes up water to boric acid (Tremain, 1998).	Y	1	Mellor's Comprehensive Treatise on Inorganic and Theoretical Chemistry, Volume V Boron, Part A: Boron-Oxygen Compounds, Longman London and New York, (1980), ISBN 0-582-46277-0, page 180-182. Tremain S.P., [redacted] 1998.	

3.2.1 Henry´s Law Constant (Pt. I-A3.2)	-	-	-	Not applicable due to low vapour pressure.	-	-	-	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 Test Guideline 101 and TNO-PML Standard Operating Procedure Q213-W-058	>97.5%	The molar extinction coefficient of the test substance could not be determined because there were no absorption maxima or minima in twice distilled water, basic of acidic medium observed.	No unusual effects were observed in running the spectra.	Y	1	Spruit WET, [redacted] 005, [redacted]	
IR	TNO-PML Standard Operating Procedure Q214-W-125; version 2 (No EC Test Guideline specified).	>97.5%	Major peaks observed at 754, 1196 and 1473 cm^{-1}.	The sample was ground in KBr powder and pressed. The test substance was recorded on an FTIR-spectrometer. The recorded FTIR-spectrum of the test substance is depicted in spectrum number ITA0003 of the report.	Y	1	Spruit [redacted] 005, [redacted]	

NMR	-	-	-	The recording of the ^{13}C NMR Spectrum of the test substance as reflected in TNO protocol no. 014.16563 dated August 23, 2004 is irrelevant due to the fact that the test substance does not contain carbon atoms.	Y	1	Spruit WET, [redacted] 2005, [redacted]	
MS	-	-	-	At TNO mass spectrometery of inorganic boron compounds, like Boric Oxide, can be done with liquid chromatography and electrospray mass spectrometry (LC-ES MS). However, earlier experience with these compounds has shown that the electrospray mass spectra do not provide any direct information on the particular boron compounds, see reports TNO-PML 2002-C041rr, -C042rr, -C043rr, -C044rr. Elecgtrospray does not ionise inorganic boron compounds in a way that allows recording of mass spectral characteristics relevant to the compounds identity and composition.	Y	1	Spruit [redacted] 005, [redacted]	

3.5 Solubility in water (IIA3.5)	-	-	Not appropriate. It is technically impossible to determine the solubility of boric oxide as a discrete species.	The performance of a water solubility study in accordance with EU Annex V test methods and OECD guidelines is considered to be technically impossible. Boric oxide reacts quickly with water to from boric acid: $B_2O_{3(s)} + 3H_2O_{(l)} \rightarrow 2H_3BO_{3(aq)}$ The EU Annex V definition of solubility is the saturation mass concentration of the substance in water at a given temperature. Given that boric oxide reacts with water it would be technically impossible to determine the saturation mass concentration of boric oxide. Any attempt to determine the solubility would in effect be measuring the solubility of boric acid. In saturated aqueous boric acid, boric oxide will immediately react with water and crystallise out as solid boric acid.	Y	1	Hoare [redacted] 2003.	X8
Water solubility 1	No data	Boric oxide 98.1 - 99.8% w/w	**result:** 22 g/l **temperature:** 20°C **pH:** 3.7 concentration: 26.6 g/l at 20°C pKa = 9.15 (at 20°C)	Boric oxide is the anhydride of boric acid (CAS No. 10043-35-3). It is hydroscopic and takes up water to form boric acid. Therefore for practical purposes one part of boric oxide is equivalent to 1.776 parts of boric acid in aqueous solution. pH of aqueous solution ranges from 6.1 at 0.056% w/w boric oxide equivalent to 3.7 at 2.66% w/w	No data	2	Mellor's Comprehensive Treatise on Inorganic & Theoretical Chemistry, Volume V Boron, Part A: Boron-Oxygen Compounds, Longman London and New York (1980), ISBN 0-582-46277-0, page 254 Boron Products and their Applications, Illustrated booklet issued by Borax Holdings Limited, Borax House, Carlisle Place, London SW1P	

				boric oxide equivalent at 20°C.			1HT. (pH). Dawber JG and D.H. Matusin, J. Chem. Soc., Faraday Trans.1, 1982, 78, 2521-2528. (pKa).	
3.6 **Dissociation constant (-)**	-	-	-	Not required.	-	-	-	X9
3.7 **Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)**	-	-	**result:** Soluble in ethanol.	-	No data	2	CRC Handbook of Chermistry and Physics, CRC Press, 2001, 82nd Edition, 4-47.	X10
3.8 **Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)**	-	-	Not required.	Boric oxide as manufactured does not contain and organic solvent.	-	-	-	

3.9 Partition coefficient n-octanol/water (IIA3.6)	-	-	Not appropriate. It is technically impossible to determine the octanol/water partition coefficient for boric oxide as a discrete species.	The performance of an octanol/water partition coefficient study in accordance with EU Annex V test methods is considered to be technically impossible. For the flask shake method, equilibrium between all interacting components of the system must be achieved, and the concentrations of the substances dissolved in the two phases must be determined. As boric oxide reacts quickly with water, it is impossible to determine the solubility of boric oxide in water or indeed to achieve and equilibrium between boric oxide$_{octanol}$/boric oxide$_{water}$. The hplc method is not applicable, as boric oxide will react with the water eluant.		-	Hoare A.M. [redacted] 2003.	X11
log Pow 1	*including effects of pH (5-9)*	Test substance: boric acid (No data on purity).	result: -0.757 temperature: 25°C	Boric oxide is the anhydride of boric acid (CAS No. 10043-35-3) and is hydroscopic taking up water to form boric acid. Therefore for practical purposes one part of boric oxide is equivalent to 1.776 parts of boric acid in aqueous solution and therefore the partition coefficient of boric acid is applicable to boric oxide.	No data	2	Barres M, Rev. Chim. Miner., 1967, 4, 803-838.	
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	-	-	-	Nearly anhydrous B_2O_3, having 20ppm water has a softening point of 300-325°C (Kirk-Othmer). Boric oxide can be heated to temperatures >1000°C without forming breakdown products.	-	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons Inc., New York, 1992, 4th Edition, Volume 4, page 369.	X12

3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	-	-	Not applicable.	Boric oxide is a non-volatile, non-flammable inorganic solid.	-	-	-	X13
3.12 Flash-point (IIA3.9)	-	-	Not applicable.	Boric oxide is a non-volatile, non-flammable inorganic solid.	-	-	-	
3.13 Surface tension (IIA3.10)	-	-	-	Boric oxide has a low surface tension.	-	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons Inc., New York, 1992, 4th Edition, Volume 4, page 369.	X14
Surface tension 1	Surface tension measurements determined with a Cenco Model No.70545 DuNuoy type Interfacial Tensiometer.	Borax tetraborate pentahydrate (~100%)	**result:** 71.0 ±0.4 mN/m **temperature:** 23°C **concentration**: 0.3g/l	-	N	2	Wurster, E.D., Surface tension of aqueous 5-mol borax solutions, US Borax Research Corporation, Technical Service Report No. 29A-1, 1963.	
3.14 Viscosity (-)	No data	No data	6.1 x 10^{10} Pa.s at 260°C. 3.9 x 10^{3} Pa.s at 500°C.	Boric oxide is a solid substance. Boric oxide becomes pourable on heating to about 500°C.	No data	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons Inc., New York, 1992, 4th Edition, Volume 4, page 369.	

3.15 **Explosive properties (IIA3.11)**	-	-	-	No explosive properties. The standard heat of formation is –1252.2 kJ.	No data	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons Inc., New York, 1992, 4th Edition, Volume 4, page 369.	X15
	-	-	-	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. Conclusion: Considering the molecular structure and the information that is available in the literature, boric oxide is not expected to have explosive properties in the sense of EC Directive 92/69/EEC.	-	1	Mak WA, 2004, [redacted]	
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	-	1	Mak WA, 2004, [redacted]	X16

				literature, boric oxide is not expected to have oxidizing properties in the sense of EC Directive 92/69/EEC.				
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	15-Sept-05
Materials and methods	Section 3.1.1. Melting point a. Two studies were summarized by the notifier without indication which study was considered as key study. Study 1 (Mellor's Comprehensive) is an encyplopedia and is given reliability 4 because no methods are described. Study 2 (Cuthbert and Mullee, 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, OECD 102). The study is given reliability 2 because the purity of the active substance is not known b. Experiments were carried out with batch number BRt 2638 [redacted] Data on the purity of the active substance and data on impurities was made available by the applicant and confirmed that the sample used is representative for the a.s. specification. d. The full reference for the key study should be stated as: [redacted]
Conclusion	No melting point found in the range 25-360 °C. Endotherms observed at 100 °C, 140 °C and 160 °C are interpreted as loss of free and crystallisation water.
Reliability	study 1 is reliability 4; study 2 is reliability 2 (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	29-Apr-05
Materials and methods	Section 3.1.2. Boiling point. a. The one study submitted (Kirk-Othmer) is an encyclopedia without any indications on methods and is given reliability 4. The encyclopedia confirmed that the boiling point was far above 360 °C. 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 25-360 °C. Phase transitions were found at 100 °C, 140 °C and 160 °C. Therefore additional data are not required.
Conclusion	A boiling point is not applicable because the melting point lies above 360 °C. Endotherms observed at 100 °C, 140 °C and 160 °C are interpreted as loss of free and crystallisation water.
Reliability	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	15-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 (Mellor's Comprehensive) is an encyclopedia and is given reliability 4 because no methods are described. Study 2 (Cuthbert and Mullee, 2003) is considered as key study by the RMS because this study was carried out under GLP according to EC method A3 (OECD 109). The study is given reliability 2 because the purity of the active substance is not known. b. Experiments were carried out with batch number BRt 2638 [redacted] Data on the purity of the active substance and data on impurities was made available by the applicant and confirmed that the sample used is representative for the a.s. specification. c. The physical state of the measured substance is a solid. d. Only the absolute density at 21.5 °C is given, whereas the relative density compared to water at 4 °C should be given. The relative density to water at 4 °C can however be calculated by dividing the absolute density with 1000.00 kg/m^3. $D^{21.5}_{4} = 1.84$. Because only two single measurements were taken, no indication of the precision can be given. e. The relative density is expressed as $D^{21.5}_{4}$ whereas it should be expressed as D^{20}_{4}. This small temperature difference is not expected to cause a large deviation and the value is considered acceptable by the RMS. f. The full reference for the key study should be stated as [redacted]
Conclusion	Relative density $D^{21.5}_{4}= 1.84$
Reliability	study 1 is reliability 4; study 2 is reliability 2 (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	29-Apr-05
Materials and methods	Section 3.2. Vapour pressure. a. Two studies were summarized by the notifier without indication which study was considered as key study. Study 1 (Meller's Comprehensive) is an encyclopedia and is given reliability 4 because no methods were described. Study 2 (Tremain, 1998) concerns experiments with boric acid and not with boric oxide. This study is given reliability 4. Therefore no reliable studies are available. Based on studies with boric acid, vapour pressure is expected to be below 10^{-5} Pa
Conclusion	Not applicable, because the melting point lies above 300 °C. At ambient temperature the vapour pressure is expected to be below 10^{-5} Pa.
Reliability	both studies 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	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 boric oxide 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	15-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. . Data on the purity of the active substance are required.
Conclusion	as indicated by the notifier
Reliability	as indicated by the notifier.
Acceptability	not acceptable. The notifier is requested to give full specification details of the batches used in the experiments i.e. active substance content.
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 15-Sept-05

Materials and methods Section 3.4 Spectra

a. One study report was submitted. The study is considered as key study by the RMS and is given reliablity of 1 because the study was carried out according to GLP and according to guidelines.

b. The study was carried out for batch number BRt3001D [redacted] The purity was reported to be >97.5%. Data on impurities are not available

c. UV/VIS spectra were recorded between 200-750 nm according to OECD 101. Test solution was 0.9516 g/L as boric oxide.

d. FTIR spectra were recorded between 400-4000 cm^{-1}. The test substance was recorded as KBr pellet. Peaks were observed at 548 (narrow), 645 (narrow), 745 (broad), 884 (narrow), 1196 (narrow), 1473 (broad), 2261 (narrow), 2362 (narrow) and 3224 (narrow) cm^{-1}.

e. A statement was given that ^{13}C-NMR spectra are not applicable, because boric oxide does not contain carbon atoms. Although ^{11}B-NMR or ^{17}O-NMR are more appropriate, these instruments are not available in most laboratories.

f. A statement was given that MS spectra from HPLC-MS with electrospray ionisation are unsuccessful because solutions of boric oxide cannot be ionised in this system.

h. Another technique which is appropriate to elucidate the structure of boric oxide is Raman spectroscopy or X-ray spectroscopy. Spectral data for these techniques are welcome. See also Mellor's Comprehensive, submitted for IIIA3.1.

i. The full reference of the newly submitted key study is: [redacted]

Conclusion No absorption maxima or minima are observed in the UV/VIS spectrum of boric oxide solution in water, basic medium or acidic medium.

FTIR spectra of boric oxide recorded as KBr pellet revealed peaks at 548 (narrow), 645 (narrow), 745 (broad), 884 (narrow), 1196 (narrow), 1473 (broad), 2261 (narrow), 2362 (narrow) and 3224 (narrow) cm^{-1}.

^{13}C-NMR spectra are not applicable, because boric oxide does not contain carbon atoms.

MS spectra could not be obtained because solutions of boric oxide could not be ionised in a HPLC-ES-MS system.

Reliability set at 1 for the key study

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	15-Sept-05
Materials and methods	Section 3.5 Water solubility. a. Four studies were summarized by the notifier. Study 1 (Hoare, 2003) is a statement why water solubility is not required. Study 2 (Mellor's Comprehensive) is an encyclopedia and refers to the solubility of boric acid. Study 3 (Borax Holdings) is a product brochure without any methods. Study 4 (Dawber and Matusin, 1982) focusses on reactions between boric acid or tetrahydroxyborate ions with polyols and is considered not relevant. All studies are given reliability 4 because no methods are described. b. The water solubility for boric oxide as such cannot be determined because boric oxide is converted into boric acid upon dissolution in water: $B_2O_3 + 3H_2O = 2B(OH)_3$. The water solubility found will be the water solubility for an equivalent amount of boric acid. Therefore, information on boric acid is copied into the present document. c. Four studies on boric acid were submitted by the notifier, of which only three studies were summarized by the notifier without indication which study was considered as key study. Study 1 (Mellor's Comprehensive) is an encyclopedia. The water solubility value of 47.2 g/L from this study was used in the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh). Because no methods are indicated, the reliability is set at 4. Study 2 (Dawber and Matusin, 1982) focusses on the dissociation constant in the presence of polyols and is not relevant. Study 2 is set at a reliability of 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 A6 (flask method) and with known purity. Study 4 (Spruit, 2005) was submitted at a later stage and contained information on solubility at different pH values. This study was not summarized by the notifier but is summarized here by the RMS. d. Although GLP was indicated for the key study (study 3), the report submitted, did not contain any authorisation signatures. The GLP claim cannot be granted, but this is considered of minor importance as the report is of sufficient quality.e.

Experiments in the key study (study 3) were carried out with batch number 225-01-442 [redacted]. Purity specification ranges from 99.0 to 100.5%. Data on impurities are not available.

f. The solubility in the key study (study 3) was determined by EC method A6 (flask method) and samples were analysed by HPLC with refractive index detection. A solution of boric acid in water gets a pH of 3.76.

g. The reference is stated wrong in the boric acid table. The full reference for the key study should be stated as: [redacted]

h. The key study determines the water solubility by dissolving the substance in water (resulting pH=3.76), whereas the effect of pH (5 to 9) must be studied. In the Kirk-Othmer encyclopedia (submitted under IIIA3.1.1, boric acid dossier) a temperature dependence of water solubility is indicated. Therefore also the effect of temperature on the water solubility must be studied.

i. A fourth study was submitted at a later stage to fulfil these data gaps and was not summarized by the notifier. The reference is not listed in the boric acid table. The full reference for this study is [redacted]

j. Although GLP was indicated for the fourth study, the report submitted, did not contain any authorisation signatures. The fourth study is considered as second key study. The GLP claim cannot be granted, but this is considered of minor importance as the report is of sufficient quality.

k. Experiments in the fourth study were carried out with batch number BRt3001B ([redacted] The purity of the active substance is given as 99.9%. Data on impurities are not available.

l. The solubility in the fourth study was determined by EC method A6 (flask method) and samples were analysed by HPLC with refractive index detection.

m. Water solubility in the first key study (study 3) was 49.2 ± 0.35 g/L at 20 ± 0.5 °C in unbuffered water, resulting in a pH of 3.76. Water solubility in the second key study (study 4) was 48.07 ± 0.83 g/L at 20 °C in unbuffered water, resulting in a pH of 3.85-4.08. The mean value for both these studies is 48.6 ± 0.90 g/L at 20 °C. Values for 10 and 30 °C are presented in the conclusions.

n. To determine the water solubility at pH=7 and 9, a Na/K phosphate buffer and tris-HCl buffer was used respectively. But upon dissolution the pH changed to 5.6-5.7 indicating insufficient buffering capacity. The molarity of the phosphate and tris buffers was not indicated, but borate itself is a very powerful buffer. Further, the solubility of boric acid is influenced by the ion-pair formation that occurs in the presence of alkali-metal ions (e.g. Na, K) . Therefore, the determination of water solubility at other pH-values is not possible and no further studies are required.

Conclusion

The water solubility for boric oxide as such cannot be determined because boric oxide is converted into boric acid upon dissolution in water: $B_2O_3 + 3H_2O = 2B(OH)_3$. The water solubility found will be the water solubility for an equivalent amount of boric acid.

1 g boric acid is equivalent to $0.5xMW_{\text{boric oxide}}/MW_{\text{boric acid}} = 0.5x69.62/61.833 = 0.563$ g boric oxide. Therefore water solubility for boric oxide is:

pH4.25-4.41: 20.4 g/L in water at 10°C, calculated from boric acid solubility.

pH 3.76-4.08: 27.2 g/L in water at 20°C, calculated from boric acid solubility.

pH 3.96-4.07: 35.2 g/L in water at 30°C, calculated from boric acid solubility.

	pH 5.60-5.69: 30.5 g/L at 20°C in Na/K-phosphate solution, calculated from boric acid solubility. pH 5.64-5.69: 35.4 g/L at 20°C in tris-HCl solution, calculated from boric acid solubility. pH 5.96 – 6.01: 37.4 g/L at 20 °C in ammonium carbonate buffer, calculated from boric acid solubility.This water solubility was calculated from experiments with boric acid. Water solubility studies at pH=5, 7, 9 are not possible, because of the strong buffering capacity of boric acid solutions and ion-pair formation in the presence of alkali-metal ions like Na, K.
Reliability	boric oxide study 1, 2, 3, 4, set at 4 boric acid study 1 (Mellor Comprehensive), set at 4. boric acid study 2 (Dawber and Matusin), set at 4. boric acid study 3 (Cordia et al., 2003), set at 1 (key study) boric acid study 4 (Spruit, 2005), 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 14-Feb-05

Materials and methods Section 3.6 Dissociation constant.

a. No data or statements submitted. The dissociation constant for boric oxide as such cannot be determined because boric oxide is converted into boric acid upon dissolution in water: $B_2O_3 + 3H_2O = 2B(OH)_3$. The dissociation constant found will be the dissociation constant for boric acid. Therefore, information on boric acid is copied into the present document.

b. 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.

----

c. The references from document IIIA6.2-A10 read across for boric oxide contained additional information on dissociation constants:

<u>Ingri, 1963</u> 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 $B \leq 0.025$ 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: $B(OH)_3 \leftrightarrow$ polynuclear anions $\leftrightarrow B(OH)_4^-$. At low boron concentrations ($B \leq 0.025$ M) the equilibrium changes into $B(OH)_3 \leftrightarrow B(OH)_4^-$.

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.

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. Because none of the peaks found was identified by the study author, 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]

----

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 boric oxide as such cannot be determined because boric oxide is converted into boric acid upon solution in water: $B_2O_3 + 3H_2O = 2B(OH)_3$. The dissociation constant found will be the dissociation constant for boric acid.

At low boron concentrations ($B \leq 0.025$ 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 ($B \leq 0.025$ 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	Reliability is set at 4 for all studies, except Ingri, 1963 set at 2.
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	25-Jan-05
Materials and methods	Section 3.7 Solubility in organic solvents. a. One study was summarized by the notifier. The study (CRC Handbook of Chemistry and Physics) was an encyclopedia and is given reliability 4. The values stated could not be found in the 1999 version of the CRC Handbook, the 2001 version was not available to the present reviewer. Data on solubility in organic solvents will not give any relevant information for the risk assessment. The critical endpoints that may be influenced by the solubility in organic solvenst were experimentally determined (e.g. log Pow)
Conclusion	No reliable data available; not required.
Reliability	reliability is set at 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	