Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	20-Sept-05
Materials and methods	Section 3.5 Water solubility, disodium tetraborate anhydrous. a. The water solubility for disodium tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid/borate upon dissolution in water: $Na_2B_4O_7 + 7\,H_2O = 2\,NaB(OH)_4 + 2\,B(OH)_3$. 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. None of the studies is considered reliable enough to be a key study by the RMS. Study 1 (Mellor's Comprehensive) refers to the water solubility of boric acid. Study 1 and study 2 (Kirk-Othmer) are encyclopediae without indication of methods or purity of substances. The reliability is set at 4 for both studies. c. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) the value of 24.8 g/L at 20 °C, pH=9.2 for disodium tetraborate unspecified is derived from study 2. The value can however not be found in this study. The data are considered not reliable by the RMS. d. The water solubility for disodium tetraborate decahydrate is equal to an equivalent amount of disodium tetraborate pentahydrate or disodium tetraborate decahydrate. Water solubility for pentahydrate is 40.06 ± 2.70 g/L at 20 ± 0.5 °C. This is equivalent to 40.06 x $MW_{anhydrous}/MW_{pentahydrate}$ = 40.06 x 201.22/291.296 = 40.06 x 0.691 = 27.7 ± 1.87 g/L. Water solubility for decahydrate is 49.74 ± 3.63 g/L at 20 ± 0.5 °C. This is equivalent to 49.74 x $MW_{anhydrous}/MW_{decahydrate}$ = 49.74 x 201.22/381.373 = 49.74 x 0.528 = 26.2 ± 1.92 g/L. Average of 27.7 g/L and 26.2 g/L is 27.0 g/L at 20 ± 0.5 °C. Deviation is sqrt ($1.87^2 + 1.92^2$) = 2.7 g/L
Conclusion	The water solubility for disodium tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid/borate upon dissolution in water: $Na_2B_4O_7 + 7\,H_2O = 2\,NaB(OH)_4 + 2\,B(OH)_3$. The water solubility found will be the water solubility for boric acid in the presence of sodium ions. The water solubility for disodium tetraborate anhydrous is equal to an equivalent amount of disodium tetraborate pentahydrate or disodium tetraborate decahydrate. Based on studies with the pentahydrate and decahydrate, water solubility is 27.0 ± 2.7 g/L at 20 ± 0.5 °C. 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 and 2 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	

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 3.6 Dissociation constant, disodium tetraborate anhydrous. 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 basic properties (pH = 9.2 for a saturated solution). b. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) it is stated that the partition coefficient for disodium tetraborate cannot be measured due to conversion into H_3BO_3 in aqueous solution. c. The dissociation constant for disodium tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid upon dissolution in water: $Na_2B_4O_7 + 7\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. 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. d. 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. --- e. The references from document IIIA6.2-A10 read across for boric oxide 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 $B \leq 0.025$ 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:

1. $B(OH)_3 + 2H_2O \leftrightarrow [B(OH)_4]^- + H_3O^+$ pKa1 = 9.0
2. $4B(OH)_3 + [B(OH)_4]^- \leftrightarrow [B_5O_6(OH)_4]^- + 6H_2O$ pKa5 = 6.8
3. $2B(OH)_3 + [B(OH)_4]^- \leftrightarrow [B_3O_3(OH)_4]^- + 3H_2O$ pKa2 = 6.8
4. $2B(OH)_3 + 2[B(OH)_4]^- \leftrightarrow [B_4O_5(OH)_4]^{2-} + 5H_2O$ pKa4 = 14.8
5. $B(OH)_3 + 2[B(OH)_4]^- \leftrightarrow [B_3O_3(OH)_5]^{2-} + 3H_2O$ pKa3 = 16.5

Borate equilibrium constants are influenced by group I metal salts (Na, K, Cs) and temperature. In the presence of NaCl, K1 becomes larger and K4 smaller as temperatures increase. With increasing size of hydrated cation (Na, K, Cs) K1, K2 and K4 increase. Maximum values of K1, K2, K3, K4 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 $[B_3O_3(OH)_4]^-$, $[B_4]^{2-}$, $[B_5]^-$ and $[B_3]^-$ 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.

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 [redacted]

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f. 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 tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid/borate upon dissolution in water: $Na_2B_4O_7 + 7\,H_2O = 2\,NaB(OH)_4 + 2\,B(OH)_3$. 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: $B(OH)_3$ ↔ polynuclear anions ↔ $B(OH)_4^-$. 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	21-Feb-05
Materials and methods	Section 3.7 Solubility in organic solvents, disodium tetraborate anhydrous. a. One study was summarized by the notifier, which is considered not reliable enough as key study by the RMS. The study (Kirk-Othmer) is an encyclopedia without any indications on methods and is given reliability 4. c. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) no data are given for disodium tetraborate anhydrous.
Conclusion	No reliable data available. However, the active will not be used in organic solvents. Critical endpoints influenced by solubility in organic solvents like the log Pow were experimentally determined.
Reliability	0
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	27-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	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	20-Sept-05
Materials and methods	Section 3.9 Partition coefficient, disodium tetraborate anhydrous. 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 tetraborate anhydrous cannot be measured because the substance breaks down to boric acid and disodium tetraborate. The RMS agrees that the partition coefficient for disodium tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid upon dissolution in water: $Na_2B_4O_7 + 7\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. 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. 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 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).

	h. In the alternate study (Barres, 1967) the log Pow value was found to be dependant upon the salt concentration in the aqueous solution and on temperature: log Pow = -0.757 in water at 25 °C log Pow = -0.742 in 2 M KCl at 25 °C log Pow = -0.561 in 3 M $NaClO_4$ at 25 °C log Pow = -0.554 in 3 M $NaClO_4$ at 35 °C It was found that in a $B(OH)_3$-$NaB(OH)_4$ or $B(OH)_3$-$KB(OH)_4$ system, undissociated boric acid was the only compound extracted into octanol. i. The value found in the key study (-1.09 ± 0.16 at 22 °C) differs from the value found in the alternate study (-0.757 ± 0.004 at 25 °C). The notifier indicates that the temperature can give an error of maximum 0.01 log-unit, but this effect may actually be somewhat larger. At least no proof is given for this statement. The difference between the two values is probably caused by differences in boron concentration (> 0.025 M in alternate study, <0.025 M in key study) and differences in the solvent (decarbonated unbuffered water in alternate study, sodium or potassium phosphate buffer in key study). j. The difference between log Pow values obtained at different temperatures, different salinity, different concentration and different analysis, is only 0.5 log Pow unit. No further tests are required. k. The reference is stated wrong in the table for boric acid. The full reference for the key study should be stated as: [redacted]
Conclusion	The partition coefficient for disodium tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid/borate upon dissolution in water: $Na_2B_4O_7 + 7\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. The partition coefficient found will be the partition coefficient for boric acid in the presence of sodium ions. log Pow = -0.561 to -1.09 at 22-25 °C, depending on the presence of metal ions (e.g sodium or potassium from buffered systems) and boron concentration..
Reliability	key study set at 1, alternate study set at 2, all others 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	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	20-Sept-05
Materials and methods	Section 3.10 Thermal stability, disodium tetraborate anhydrous. a. The notifier submitted one study (Kirk-Othmer) giving a description that disodium tetraborate anhydrous is the most stable form compared to hydrated forms of disodium tetraborate. This study is an encyclopedia and is given reliability of 4 because no methods were described and no purity data are indicated. b. Based on the melting point study (section A3.1.1) disodium tetraborate anhydrous is stable up to 525/527 °C. At this temperature a phase transition occurs. A melting point is found at 737 °C. Therefore, disodium tetraborate anhydrous is considered stable under the conditions normally required for a storage stability test (14 days at 54-55 °C, OECD guideline 113). No further studies are required.
Conclusion	Disodium tetraborate anhydrous is stable up to 525/527 °C. At this temperature a phase transition occurs. A melting point is found at 737 °C.
Reliability	reliability 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	

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 3.11 Flammability, disodium tetraborate anhydrous. a. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) it was concluded that disodium tetraborate is not flammable. Background information is however not available.
Conclusion	no reliable data available. However, since the a.s. is known for its flame retardant properties it is not expected that the tetraborates are (highly) flammable or self-igniting. No further data is considered 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	21-Feb-05
Materials and methods	Section 3.12 Flash point, disodium tetraborate anhydrous. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) it was concluded that flash point is not applicable for solids.
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	15-Feb-05
Materials and methods	Section 3.13 Surface tension, disodium tetraborate anhydrous. a. The notifier refers to disodium tetraborate pentahydrate. The notifier submitted one study (Wurster, 1963) where disodium tetraborate pentahydrate was dissolved in water. The study is considered not reliable enough to be a key study by the RMS. The study was not carried out according to GLP nor according to EC guidelines. Purity data are not indicated. The study can be used as indication study (reliability 4). b. For a 3% (w/v) solution of disodium tetraborate pentahydrate, a surface tension of 69.5-71.0 dynes/cm or mN/m was found at 23-24 °C, slightly lower than the surface tension for water (72.8 at 20 °C). The surface tension for a solution of disodium tetraborate pentahydrate is considered to be identical to the surface tension for an equivalent solution of disodium tetraborate anhydrous or disodium tetraborate decahydrate. Surface tension is considered not applicable for inorganic substances. No further data are required.
Conclusion	The surface tension for disodium tetraborate anhydrous as such cannot be determined because disodium tetraborate anhydrous is converted into boric acid/borate upon dissolution in water: $Na_2B_4O_7 + 7\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. The surface tension found will be the surface tension for boric acid in the presence of sodium ions. Surface tension is considered not applicable for inorganic substances. Disodium tetraborate anhydrous is an inorganic substance and the surface tension of a solution in water will be slightly lower than the surface tension for water (72.8 mN/m at 20 °C).
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	

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 3.15 Explosive properties, disodium tetraborate anhydrous. a. The notifier submitted a statement (Mak, 2004) and is given reliability of 4 because no methods are described. The statement that disodium tetraborate anhydrous contains no reactive groups is acceptable to show that disodium tetraborate anhydrous has no explosive properties and testing according to EC method A14 is not required. b. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) it was concluded that disodium tetraborate is not explosive. Background information is however not available.
Conclusion	as indicated by the notifier
Reliability	reliability is 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	21-Feb-05
Materials and methods	Section 3.16 Oxidizing properties, disodium tetraborate anhydrous. a. The notifier submitted a statement (Mak, 2004) and is given reliability of 4 because no methods are described. The statement that disodium tetraborate anhydrous contains no reactive groups is acceptable to show that disodium tetraborate anhydrous has no oxidizing properties and testing according to EC method A17 is not required. b. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) it was concluded that disodium tetraborate is not oxidizing. Background information is however not available.
Conclusion	as indicated by the notifier.
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	

Evaluation by Competent Authorities	
	Use separate "evaluation boxes" to provide transparency as to the comments and views submitted
	EVALUATION BY RAPPORTEUR MEMBER STATE
Date	03-June-2008
Materials and methods	Section 3.17 Reactivity towards container material. It should be noted that polypropylene becomes brittle at low temperatures. Storage at low temperatures in polypropylene should therefore be avoided.
Conclusion	-
Reliability	0
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	

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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	-	Disodium tetraborate-unspecified	**result:** 742.5°C	The two hydrated forms of disodium tetraborate do not melt as such. When disodium tetraborate decahydrate is heated (in an open space) above about 62°C, it gradually loses water of crystallisation, first forming the pentahydrate, Na2B4O.5H2O, and on further heating forms anhydrous disodium tetraborate, Na2B4O7, the crystal form of which melts at 742°C.	No data	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons Inc., 1992, 4th Edition, Volume 4, page 382.	
Melting pt. 2	ASTM E 537-76 (Differential Thermal Analysis).	101.7-103.1%	**result:** 737°C.	An endothermal peak is observed at 131/131°C, probably due to the loss of water. Due to a phase transition an exothermal peak is observed at 524/527°C. The water free borax melts eventually at 739/736°C.	Y	1	Cordia J [redacted], 2003,	
3.1.2 Boiling point	-	-	Not applicable.	Not applicable for disodium tetraborate pentahydrate as this loses water of crystallisation on heating.	-	-	-	X2
3.1.3 Bulk density/ relative density								X3

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
Bulk/rel. density 1	-	Disodium tetraborate pentahydrate	Relative density = 1.81	-	No data	2	Borax internal product spec.	
Bulk/rel. density 2	Test Guideline A.3 of EC Directive 92/69/EEC	101.7-103.1%	Relative density = 1.860 ± 0.008	-	Y	1	Cordia J.A. [redacted] 2003,	
3.2 Vapour pressure (IIA3.2)	-	-	Not applicable.	The vapour pressure value for both disodium tetraborate pentahydrate and disodium tetraborate is negligible at ambient temperatures. A vapour pressure study on Boric acid (Tremain et al., 1998) indicated a negligible vapour pressure of 0.000000099 hPa at 25°C and on disodium octaborate tetrahydrate 0.000000000099 hPa at 25°C (Howard et al., 1995) Therefore no further testing is required.	Y	1	Tremain SP, [redacted] 1998 Howard R, [redacted] 1995,	X4
3.2.1 Henry´s Law Constant (Pt. I-A3.2)	-	-	-	Not applicable to materials of low vapour pressure.	-	-	-	
3.3 Appearance (IIA3.3)								X5
3.3.1 Physical state			Solid					
3.3.2 Colour			White					

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
3.3.3 Odour	Odourless							
3.4 Absorption spectra (IIA3.4)								X6
UV/VIS	OECD Guideline 101 and TNO-PML S.O.P. Q213-W-058.	101.7-103.1%	Molar extinction coefficient could not be determined.	No unusual effects were observed in running the spectra. The molar extinction coefficient could not be determined because there were no district absorption maximum or minimum found in a neutral, basic or acidic medium.	Y	1	Cordia J.A. [redacted] 2003,	
IR	TNO-PML S.O.P. Q214-W-125 version 2.	101.7-103.1%	Major peaks observed at 826, 946, 1003, 1131, 1276 and 1472 cm^{-1}.	The sample was ground in KBr powder and pressed. The test substance was recorded on an FTIR-spectrometer.	Y	1	Cordia J.A. [redacted] 003,	
NMR	-	-	-	The recording of the ^{13}C NMR Spectrum of the test substance as reflected in TNO protocol no. 014.16589 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,	
MS	TNO-PML S.O.P. Q214-W-130.	101.7-103.1%	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 eluant and dissolution of the compounds in water or eluant. No signals characteristic of borium containing material.	Y	1	Cordia J.A. [redacted] , 2003,	

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
3.5 Solubility in water (IIA3.5)	*including effects of pH (5-9)*							X7
Water solubility 1	No data	No data	**result:** 35.9 g/l **temperature:** 20°C **pH:** 9.2 **Concentration:** 35.9 g/l at 20°C.	pH remains unchanged over a wide concentration range. Description: soluble (1000-10000 mg/l).	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. (Solubility) Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons, Inc., New York, 1992, 4th Edition, Volume 4, pages 381-386. (pH)	
Water solubility 2	Test Guidleine A.6 of EC Directive 92/69/EEC and TNO-PML S.O.P. Q213-W-036.	101.7-103.1%	**result:** 40.06 ± 2.70 g/l **temperature**: 20.0 ± 0.5°C. **pH**: 9.66	Average water solubility value given. The difference between the determined water solubility value and the literature value (37.4 g/l) is probably due to the fact that the solubility of the test substance is based on a saturated solution made up from the test substance, but the solution is actually inequilibrium with borax decahydrate crystals, not crystals of the test substance.	Y	1	Cordia J.A. [redacted] 003,	
3.6 Dissociation constant (-)	-	-	Not required.	*Only if additional data are required (see BPD, TNsG)*	-	-	-	X8
3.7 Solubility in organic solvents, including	No data	No data	**result:** 98.4 g/l **temperature:**	Solubility in diethylene glycol	N	2	Product Profile Neobor, Borax	X9

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
the effect of temperature on solubility (IIIA3.1)			25°C	Description: soluble (1000-10000 mg/l).			Europe, PP2-JH1-3-EU	
	No data	No data	**result:** 166.9 g/l **temperature:** 25°C	Solubility in methanol Description: soluble (1000-10000 mg/l).	N	2	Product Profile Neobor, Borax Europe, PP2-JH1-3-EU	
	No data	No data	**result:** 215.3 g/l **temperature:** 25°C	Solubility in propylene glycol. Description: soluble (1000-10000 mg/l).	N	2	Product Profile Neobor, Borax Europe, PP2-JH1-3-EU	
	No data	No data	**result:** 306.6 g/l **temperature:** 25°C	Solubility in ethylene glycol Description: soluble (1000-10000 mg/l).	N	2	Product Profile Neobor, Borax Europe, PP2-JH1-3-EU	
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)*	-	-	-	X10

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
3.9 Partition coefficient n-octanol/water (IIA3.6)	-	-	Not applicable.	The partition coefficient of disodium tetraborate (anhydrous, pentahydrate and decahydrate) in n-octanol/water cannot be measured accurately, because in aqueous solution sodium tetraborates are converted substantially into undissociated boric acid, H3BO3.	-	-	Barres M, Rev. Chim. Miner., 1967, 4, 803-838; Chem. Abstr.,1968,69, 30628	X11
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	-	-	-	Standard heat of formation is –4.7844 MJ/mol. Borax pentahydrate is reversibly converted to an amorphous dihydrate at 88°C and 0.26 kPa. Thermogravimetric analyses show that 2.75 moles of water are lost on heating to 140°C.	-	2	Kirk-Othmer Encyclopedia of Chemical Technology, John Wiley & Sons, Inc., New York, 1992, 4th Edition, Volume 4, pages 385.	X12
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	-	-	Non flammable.	Disodium tetraborates (anhydrous, pentahydrate and decahydrate) are non-flammable solids (flammability classification U.S.A. 29CFR 1920.1200).	-	-	-	X13
3.12 Flash-point (IIA3.9)	-	-	Test not applicable.	Sodium tetraborates (anhydrous, pentahydrate and decahydrate) are non-flammable inorganic solids.	-	-	-	

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
3.13 Surface tension (IIA3.10)								X14
Surface tension 1	Surface tension measurements determined with a Cenco Model No.70545 DuNuoy type Interfacial Tensiometer.	Borax tetraborate pentahyd-rate (~100%)	**result:** 71.0 ±0.4 mN/m **temperature:** 23°C **concentration**: 0.3g/l	-	N	2	Wurster, E.D., [redacted], 1963.	
3.14 Viscosity (-)	-	-	Not applicable.	Disodium tetraborate pentahydrate is a solid substance.	-	-	-	
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. Conclusion: Considering the molecular structure and the information that is available in the literature, disodium tetraborate pentahydrate is not expected to have explosive properties in the sense of EC Directive 92/69/EEC.	-	1	Mak WA, 2004, [redacted]	X15
3.16 Oxidizing properties	-	-	-	In principle, inorganic substances	-	1	Mak WA, 2004, [redacted]	X16

Section A3 Physical and Chemical Properties of Active Substance - *Disodium tetraborate pentahydrate*

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
(IIA3.12)				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 tetraborate pentahydrate is not expected to have oxidizing properties in the sense of EC Directive 92/69/EEC.			[redacted]	
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	20-Sept-05
Materials and methods	Section 3.1.1. Melting point, disodium tetraborate pentahydrate a. Two studies were summarized by the notifier without indication which study was considered as key study. Study 1 (Kirk-Othmer) is an encyclopedia. The melting point value of 742 °C 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 indications on methods were available, the study is given reliability 4. The study can however be 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 A1 (= ASTM E 537-1) and with known purity. b. Although GLP was indicated for study 2, the report submitted, did not contain any authorisation signatures. An authorised report is not required as there is no hard GLP requirement. c. Experiments in the key study were carried out with batch number BRT 2463 ([redacted] Purity specification ranges from 101.7%-103.1%. The purity of disodium tetraborate pentahydrate in the key study complies with the minimum purity indicated in chapter IIIA2.7 for both manufacturers. However, minimum and maximum purity cannot be higher than 100%. Data on impurities are not available. d. In the key study differential thermal analysis (DTA) was used in the temperature range 25-1000 °C. e. The melting point value found in study 1 (Kirk-Othmer) for disodium tetraborate anhydrous was 742.5 °C, which confirms the value found in the key study. f. The reference is stated wrong in the table. The full reference for the key study should be stated as: [redacted]
Conclusion	Not applicable. No melting point can be defined because of decomposition of the active substance. When disodium tetraborate pentahydrate is heated, it gradually loses water of crystallisation, forming disodium tetraborate anhydrous, $Na_2B_4O_7$. An endothermal peak is observed at 131 °C, probably due to the loss of water. Due to a phase transition an exothermal peak is observed at 524/527°C. The crystal form of $Na_2B_4O_7$ melts at 737°C.
Reliability	study 1 is reliability 4; study 2 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	29-Apr-05
Materials and methods	Section 3.1.2. Boiling point, disodium tetraborate pentahydrate. That a boiling point is not applicable, can be deduced from the melting point study (section A3.1.1) where a melting point was found at 737 °C. At 131°C probably hydration water is lost and at 525/527 °C a phase transition is found. Therefore additional data are not required.
Conclusion	A boiling point is not applicable because of decomposition of the active substance. When disodium tetraborate pentahydrate is heated, it gradually loses water of crystallisation, forming disodium tetraborate anhydrous, $Na_2B_4O_7$. An endothermal peak is observed at 131 °C, probably due to the loss of water. Due to a phase transition an exothermal peak is observed at 524/527°C. The crystal form of $Na_2B_4O_7$ melts at 737°C.
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	20-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 sheet with internal product specifications which was not submitted and is given reliability 4. The value of 1.81 at 20 °C is the same value as stated in the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh). The data are considered not reliable by the RMS. 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. Although GLP was indicated for study 2, the report submitted, did not contain any authorisation signatures. An authorised report is not required.as there is not hard GLP requirement. c. Experiments in the key study were carried out with batch number BRT 2463 [redacted] Purity specification ranges from 101.7%-103.1%. The purity of disodium tetraborate pentahydrate in the key study complies with the minimum purity indicated in chapter IIIA2.7 for both manufacturers. However, minimum and maximum purity cannot be higher than 100%. Data on impurities are not available. d. The physical state of the measured substance is a solid. The method used was a multi-volume pycnometer. Experiments were carried out at 22±1 °C. e. 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. f. The reference is stated wrong in the table. The full reference for the key study should be stated as: [redacted]
Conclusion	Relative density $D^{22}_4 = 1.860 \pm 0.008$
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	29-Apr-05
Materials and methods	Section 3.2. Vapour pressure, disodium tetraborate pentahydrate. The notifier submitted two studies where the vapour pressure has been determined for boric acid (Tremain, 1998) or for disodium octaborate tetrahydrate (Howarth et al., 1995). Both studies are considered not relevant by the RMS for disodium tetraborate anhydrous. Both studies are set at reliability of 4.
Conclusion	Not applicable. At ambient temperature the vapour pressure is expected to be less than 10^{-5}Pa.
Reliability	study 1 and 2, 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, disodium tetraborate pentahydrate 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 tetraborate pentahydrate 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	20-Sept-05
Materials and methods	Section 3.3 Appearance, disodium tetraborate pentahydrate a. Physical state, color and odour is stated without specification of the purity of the active substance, impurities present, temperature and pressure. b. Physical state corresponds with data in the RAR for boric acid and disodium tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh).
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	20-Sept-05
Materials and methods	Section 3.4 Spectra, disodium tetraborate pentahydrate a. Two studies were submitted. Study 1 contains data and is considered as key study by the RMS, because GLP was indicated and data were obtained according to guidelines. Study 2 is a statement 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 not required as there is no hard GLP requirement. c. Experiments in the key study were carried out with batch number BRT 2463 [redacted] Purity specification ranges from 101.7%-103.1%. The purity of disodium tetraborate pentahydrate in the key study complies with the minimum purity indicated in chapter IIIA2.7 for both manufacturers. However, minimum and maximum purity cannot be higher than 100%. Data on impurities are not available. d. UV/VIS spectrum was 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. The UV/VIS spectrum of disodium tetraborate pentahydrate is equal to the UV/VIS spectrum of disodium tetraborate anhydrous, which was recorded between 200-750 nm. No absorption maximum or minimum was found. Therefore no additional data are needed. e. FTIR spectra were recorded between 400-4000 cm^{-1}. Peaks were observed at 464 (narrow), 507 (narrow), 710 (narrow), 826 (narrow), 946 (narrow), 1003 (broad) 1079 (narrow), 1131 (narrow), 1276 (narrow), 1347-1472 (broad), 1661 (narrow), 2438 (narrow), 2611 (narrow), 3356 (broad) cm^{-1}. f. A statement was given that ^{13}C-NMR spectra are not applicable, because disodium tetraborate pentahydrate does not contain carbon atoms. 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 tetraborate pentahydrate 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 maxima or minima are observed in the UV/VIS spectrum of disodium tetraborate pentahydrate solution in the range 190-750 nm in water, basic medium or acidic medium. FTIR spectra of disodium tetraborate pentahydrate recorded as KBr pellet revealed peaks at 464 (narrow), 507 (narrow), 710 (narrow), 826 (narrow), 946 (narrow), 1003 (broad) 1079 (narrow), 1131 (narrow), 1276 (narrow), 1347-1472 (broad), 1661 (narrow), 2438 (narrow), 2611 (narrow), 3356 (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 tetraborate pentahydrate 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	20-Sept-05
Materials and methods	Section 3.5 Water solubility, disodium tetraborate pentahydrate. a. Water solubility for disodium tetraborate pentahydrate as such cannot be determined because disodium tetraborate pentahydrate is converted into boric acid upon dissolution in water: $Na_2B_4O_7.5H_2O + 2\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. The water solubility found will be the water solubility for boric acid in the presence of sodium ions. b. 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 refers to the water solubility of boric acid. Study 2 (Kirk-Othmer) is an encyclopedia without method description or purity indication. Study 1 and 2 are 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. c. Although GLP was indicated for the key study, the report submitted, did not contain any authorisation signatures. An authorised report is required to support GLP claims. d. Experiments in the key study were carried out with batch number BRT 2463 [redacted] Purity specification ranges from 101.7%-103.1%. The purity of disodium tetraborate pentahydrate in the key study complies with the minimum purity indicated in chapter IIIA2.7 for both manufacturers. However, minimum and maximum purity cannot be higher than 100%. 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. A saturated solution of disodium tetraborate pentahydrate in water gets a pH of 9.66. f. The effect of pH (5 to 9) and temperature on the solubility was not 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. Effect of temperature on the solubility is however required. g. The reference is stated wrong in the table. The full reference for the key study should be stated as: [redacted] h. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) the value of 35.9 g/L at 20 °C, pH=9.2 for disodium tetraborate pentahydrate is derived from study 1 and 2. This value could however not be found in this study. The data are considered not reliable by the RMS. i. The water solubility for disodium tetraborate pentahydrate is equal to an equivalent amount of disodium tetraborate anhydrous or disodium tetraborate decahydrate. No reliable experiments were carried out for disodium tetraborate anhydrous. For disodium tetraborate decahydrate a water solubility of 49.74 g/L was found. This is equivalent to 49.74 x $MW_{pentahydrate}/MW_{decahydrate}$ = 49.74 x 291.296/381.373 = 49.74x0.764=37.99 g/L. The actual value found was 40.06 g/L.

Conclusion	Water solubility for disodium tetraborate pentahydrate as such cannot be determined because disodium tetraborate pentahydrate is converted into boric acid upon dissolution in water: $Na_2B_4O_7.5H_2O + 2\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. The water solubility found will be the water solubility for boric acid in the presence of sodium ions. Water solubility is 40.06 ± 2.70 g/L at 20.0 ± 0.5 °C 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. Temperature dependence of the solubility in water is not considered an issue as the solubility is already very high.
Reliability	study 1 (Mellor Comprehensive), set at 4. study 2 (Dawber and Matusin), set at 4. study 3 (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	21-Feb-05
Materials and methods	Section 3.6 Dissociation constant, disodium tetraborate pentahydrate. 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 basic properties (pH = 9.66 for a saturated solution). b. In the RAR for boric acid and tetraborate (d.d. 17 December 2003, document TR417+423_1203_env_hh) it is stated that the partition coefficient for disodium tetraborate cannot be measured due to conversion into H_3BO_3 in aqueous solution. c. The dissociation constant for disodium tetraborate pentahydrate as such cannot be determined because disodium tetraborate pentahydrate is converted into boric acid upon dissolution in water: $Na_2B_4O_7.5H_2O + 2H_2O = 2NaB(OH)_4 + 2B(OH)_3$. 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. d. 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. --- e. The references from document IIIA6.2-A10 read across for the disodium tetraborates 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: $B(OH)_3 \leftrightarrow$ 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:

1. $B(OH)_3 + 2H_2O \leftrightarrow [B(OH)_4]^{-} + H_3O^{+}$ pKa1 = 9.0
2. $4B(OH)_3 + [B(OH)_4]^{-} \leftrightarrow [B_5O_6(OH)_4]^{-} + 6H_2O$ pKa5 = 6.8
3. $2B(OH)_3 + [B(OH)_4]^{-} \leftrightarrow [B_3O_3(OH)_4]^{-} + 3H_2O$ pKa2 = 6.8
4. $2B(OH)_3 + 2[B(OH)_4]^{-} \leftrightarrow [B_4O_5(OH)_4]^{2-} + 5H_2O$ pKa4 = 14.8
5. $B(OH)_3 + 2[B(OH)_4]^{-} \leftrightarrow [B_3O_3(OH)_5]^{2-} + 3H_2O$ pKa3 = 16.5

Borate equilibrium constants are influenced by group I metal salts (Na, K, Cs) and temperature. In the presence of NaCl, K1 becomes larger and K4 smaller as temperatures increase. With increasing size of hydrated cation (Na, K, Cs) K1, K2 and K4 increase. Maximum values of K1, K2, K3, K4 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 $[B_3O_3(OH)_4]^{-}$, $[B_4]^{2-}$, $[B_5]^{-}$ and $[B_3]^{-}$ 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.

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 [redacted]

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.

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f. 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 tetraborate pentahydrate as such cannot be determined because disodium tetraborate pentahydrate is converted into boric acid upon dissolution in water: $Na_2B_4O_7.5H_2O + 2\ H_2O = 2\ NaB(OH)_4 + 2\ B(OH)_3$. The dissociation constant found will be the dissociation constant for boric acid in the presence of sodium ions.

At low boron concentrations ($B \leq 0.025$ 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.