EUROPEAN CHEMICALS AGENCY

Helsinki, 19 September 2017

Addressee: [redacted]

Decision number: CCH-D-2114372099-41-01/F
Substance name: C14-18 alpha-olefin epoxide, reaction products with boric acid
List number: 939-580-3
CAS number: NS
Registration number: [redacted]
Submission number: [redacted]
Submission date: 01.09.2016
Registered tonnage band: 100-1000T

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (the 'REACH Regulation'), ECHA requests you to submit information on

1. **Name or other identifier of the substance (Annex VI, Section 2.1.) of the registered substance;**

2. **Description of the analytical methods (Annex VI, Section 2.3.7.) on the registered substance;**

3. **Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.; test method: EU B.26./OECD TG 408) in rats with the registered substance;**

4. **Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method: EU B.31./OECD TG 414) in a first species (rat or rabbit), oral route with the registered substance;**

5. **Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.; test method: Fish, early-life stage (FELS) toxicity test, OECD TG 210) with the registered substance;**

6. **Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.; test method: Aerobic mineralisation in surface water – simulation biodegradation test, EU C.25./OECD TG 309) with the registered substance;**

7. **Soil simulation testing (Annex IX, Section 9.2.1.3.; test method: Aerobic and anaerobic transformation in soil, EU C.23./OECD TG 307) with the registered substance;**

8. **Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method: Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24./OECD TG 308) with the registered substance;**

9. **Identification of degradation products (Annex IX, 9.2.3.; test method: Aerobic mineralisation in surface water – simulation biodegradation test, EU C.25./OECD TG 309) of the registered substance;**

10. **A revised PBT and vPvB assessment including PBT and vPvB assessment for the relevant constituents of the substance (including impurities) and for the relevant degradation products (Annex I, Section 4.).**

You may adapt the testing requested above according to the specific rules outlined in Annexes VI to X and/or according to the general rules contained in Annex XI of the REACH Regulation. In order to ensure compliance with the respective information requirement, any such adaptation will need to have a scientific justification, referring and conforming to the appropriate rules in the respective Annex, and an adequate and reliable documentation.

You are required to submit the requested information in an updated registration dossier by **28 September 2020**. You shall also update the chemical safety report, where relevant. The timeline has been set to allow for sequential testing.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2. Advice and further observations are provided in Appendix 3.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, shall be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under http://echa.europa.eu/regulations/appeals.

Authorised[1] by Kevin Pollard, Head of Unit, Evaluation E1

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

Appendix 1: Reasons

1. Name or other identifier of the substance (Annex VI, Section 2.1.)

Pursuant to Article 10(a)(ii) of the REACH Regulation, the technical dossier shall contain information on the identity of the substance as specified in Annex VI, Section 2 of the REACH Regulation. In accordance with Annex VI, Section 2 the information provided shall be sufficient to enable the identification of the registered substance.

ECHA notes that you have identified the registered substance as of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). Information required to be provided according to Annex VI section 2.1 of the REACH Regulation on the naming of UVCB substances such as the registered substance shall consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process, as indicated in chapter 4.3 of the Guidance for identification and naming of substances under REACH and CLP (Version: 2.1, May 2017) - referred to as "the SID Guidance" thereinafter.

You have provided a chemical/IUPAC name "C14-18 alpha-olefin epoxide, reaction products with boric acid" for your substance. This name would suggest that [redacted] are present as constituents of your substance. However, the compositional information included in section 1.2 ("legal entity composition of the substance") refer to the [redacted] only. Furthermore, the composition of the starting material provided in the description of the manufacturing process included in section 1.2 indicates that the starting [redacted]. In fact the analysis of the starting materials included in section 1.4 reveals that the [redacted] content of the registered substance is [redacted]% while the other [redacted] lengths are present at very low concentrations ([redacted] were not found).

Therefore the IUPAC name "C14-18 alpha-olefin epoxide, reaction products with boric acid" is not representative for the registered substance, as it does not reflect its composition in terms of the carbon chain lenghts present.

In line with REACH Annex VI, section 2.1 you are requested to revise the chemical/IUPAC name of your substance such that it is consistent with the composition of the substance and the composition of the starting material.

The revised chemical name shall be reported in the IUPAC name field in IUCLID section 1.1. In case the current identifiers are not appropriate to describe the registered substance, you should not remove or modify at this stage the chemical identifiers (including the List number 939-580-3) for technical reasons, the registration being linked to that List number in REACH-IT. To ensure unambiguous identification of the registered substance, you should however indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The list number 939-580-3 currently assigned does not specifically correspond to the registered substance. This identifier cannot be modified or deleted at this stage in the present registration update for technical reasons". You should also specify, in the same "Remarks" field, any available and appropriate EC number for the substance.

Any available CAS entry for the registered substance should be reported under the "CAS information" header of the reference substance in IUCLID section 1.1.
You should note that ECHA has established a process, subject to certain conditions, enabling registrants to adapt the EC identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned.

Pending the resolution of the non-compliances addressed in the present decision, any possible adaptation of the identifier can only become effective once ECHA is in a position to establish unambiguously the identity of the substance intended to be covered by you with this registration. Should the information submitted by you as a result of the present decision enable ECHA to identify the substance unambiguously and result in a need to modify the identifier of the substance, the process of adapting the identifier will be considered relevant. In that case, ECHA will inform you in due time as to when and how the identifier adaptation process shall be initiated.

In any case, you should note that the application of the process of adapting the identifier does not affect your obligation to fulfil the requirements specified in this decision.

2. Description of the analytical methods (Annex VI, Section 2.3.7.)

Pursuant to Article 10(a)(ii) of the REACH Regulation, the technical dossier shall contain information on the identity of the substance as specified in Annex VI, Section 2 of the REACH Regulation. In accordance with Annex VI, Section 2 the information provided shall be sufficient to enable the identification of the registered substance.

According to Annex VI, section 2.3.7. of the REACH Regulation, a registration dossier shall report a description of the analytical methods or the appropriate bibliographic references for the identification of the substance and where appropriate for the identification of impurities and additives. The reporting shall be given in sufficient detail that the methods may be reproduced.

You have provided in section 1.4 of the dossier a set of spectral data to prove the identity of the registered substance as well as the Gel Permeation Chromatography (GPC) analysis to quantify the constituents of the registered substance and Gas Chromatography (GC) analysis to determine the carbon chain length distribution of the oxiraine chains. The proposed structures of the main constituents were included in the table with a remark "Proposed structures were generated by MRMG based on knowledge of the reaction chemistry of boron containing compounds" (attachment [redacted]).

However, there is no further information on the "reaction chemistry of boron containing compounds" in form of for instance publically available literature of studies performed for similar systems provided. Hence, it is not clear how the composition of the registered substance was derived.

You should therefore provide details on the reaction chemistry and /or theoretical assumptions used to derive the composition of the registered substance.

As for the reporting of the data in the registration dossier, the information should be attached in IUCLID section 1.4. The information shall be sufficient for the methods to be reproduced and shall therefore include complete details of the experimental protocol followed, the calculation made and the results obtained.

3. Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.)

Pursuant to Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

A "sub-chronic toxicity study (90 day)" is a standard information requirement as laid down in Annex IX, Section 8.6.2. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

In the technical dossier you have provided a study record for a "combined repeated dose toxicity study with the reproduction/developmental toxicity screening test" (test method: OECD TG 422) by the oral route. You have also sought to adapt this information requirement by provided the following justification for the adaptation:

"A 90-day repeat dose study by the oral route is scientifically unjustified. The substance is a UCVB with the majority of components in the molecular weight range of 284 - 853 gm/mol. The substance is slightly soluble in water (0.17 mg/L), with a relatively high octanol/water partition coefficient (log Pow > 9.4) and a low vapour pressure (0.009Pa).

Under the test conditions, the NOAEL of test item was 500 mg/kg bw/day based on the lower mean food consumption and granulomatous inflammation of the mesenteric lymph node in the males and females at 1000 mg/kg bw/day in rats. Classification for repeat dose effects via the oral route is not suggested as there are no effects seen at 500 mg/kg bw/day and those at 1000 were non-adverse and reversible.

In the absence of adverse effects at the limit of classification and in respect of the reversible effects at the limit dose for this type of study in combination with the low potential for absorption via the major routes of exposure (dermal and inhalation) further investigations of systemic toxicity for longer dosing periods via the oral route are not considered scientifically justified."

While you have not explicitly claimed an adaptation, you have provided information that could be interpreted as an attempt to adapt the information requirement according to Annex IX, Section 8.6.2., column 2. Thus, the 90 day sub-chronic toxicity study would not need to be conducted if "*the substance is unreactive, insoluble and not inhalable and there is no evidence of absorption and no evidence of toxicity in a 28-day 'limit test', particularly if such a pattern is coupled with limited human exposure*".

ECHA notes that the OECD TG 422 screening study you have provided does not provide the information required by Annex IX, Section 8.6.2., because the exposure duration is less than 90 days.
Furthermore, ECHA notes that your adaptation does not meet the specific rules for adaptation of Annex IX, Section 8.6.2., column 2 for the following reasons:

- The substance is not insoluble.
- It has not been demonstrated that the substance is not absorbed. On the contrary the Expert statement by [redacted] (2016) reported under developmental toxicity discusses metabolism of absorbable components of your substance.

- There are signs of systemic toxicity in the OECD TG 422 screening study in terms of changes in clinical chemistry (such as higher mean alanine aminotransferase and higher urea nitrogen values for males in the 1000 mg/kg bw/day) and granulomatous infiltration of the mesenteric lymph nodes were noted at an exposure of 1000 mg/kg bw/day. The latter finding, together with decreased body weights of the animals at this exposure level, was the basis for the NOAEL of 500 mg/kg bw/day. According to the technical dossier the granulomatous infiltration was not fully reversible as you indicate in the adaptation justification. In addition, the substance has been classified for skin sensitisation.
- While the exposure in general may be regarded as not high, there are scenarios where RCRs are about 0.5. Thus, you have not demonstrated that there is limited human exposure and this condition is not met.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you question that a subchronic toxicity study according to OECD TG 408 as requested by ECHA would give new information to the risk assessment of the registered substance but would result in unnecessary use of vertebrate animals. Your main arguments are that

- *"the RCR values are currently very low and favourable and a 90 day study would not change the overall demonstration of safe use"*;
- using an uncertainty factor of 3 *"to estimate the 90 day NOAEL from the existing OECD TG 422 shows that the predicted 90 day results would provide no new information nor change anything in the dossier or risk assessment"*;
- *"extending the exposure duration does not necessarily lead to more severe results. In fact,* [redacted] *has experience in running both 28 day and 90 day studies for a borate compound similar to the substance in question herein, and the 90 day NOAEL (750 mg/kg/d) was in fact higher /more favourable than the 28 day NOAEL (500 mg/kg/d). This provides a further line of arguments that no new information would be gained for this risk assessment when existing 422 study is so favourable"*; and
- *"the OECD 422 study provided in the dossier used 12 (low and mid dose groups) to 17 (high dose group) animals per dose group, and the 90 day study uses 10 per dose group"* and that the *"vast majority"* of endpoints and parameters of the OECD 422 study relevant to derive risk values are covered.

ECHA acknowledges that the investigations performed in the provided OECD TG 422 study cover most of the parameters required in the 90-day study according to OECD TG 408. However, the exposure duration in your OECD TG 422 was 28 days for males and 53 days for females. ECHA acknowledges your comment that you expect no gain for risk assessment with a study of 90 day exposure duration based on a *"borate compound similar to the substance in question"*. However, you did not support this claim with justification and factual evidence. More specifically, you did not provide a justification on the similarity of the substances and you did not provide detailed information to compare the toxicity profile (including type of toxic effects observed) of those substances with respect to the endpoint in question.
In the absence of such information, it is not possible to assure that the prolonged exposure duration of a 90-day study would not have an impact on hazard identification and risk assessment.

Therefore, your adaptation of the information requirement is currently rejected.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does currently not meet the information requirement. Consequently, there is an information gap and it is necessary to provide information for this endpoint.

ECHA has evaluated the most appropriate route of administration for the study. Based on the information provided in the technical dossier and/or in the chemical safety report, ECHA considers that the oral route - which is the preferred one as indicated in ECHA Guidance on information requirements and chemical safety assessment (version 6.0, July 2017) Chapter R.7a, section R.7.5.4.3 - is the most appropriate route of administration. More specifically, even though the information indicates that human exposure to the registered substance by the inhalation route is likely, the available oral study indicates a concern for systemic toxicity as described above that requires further information on repeated dose toxicity by the oral route. Hence, the test shall be performed by the oral route using the test method EU B.26./OECD TG 408.

According to the test method EU B.26./OECD TG 408 the rat is the preferred species. ECHA considers this species as being appropriate and testing should be performed with the rat.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Repeated dose 90-day oral toxicity study (test method: EU B.26./OECD TG 408) in rats.

Note to the registrant: ECHA also acknowledges your proposal to perform the 90-day repeated dose oral toxicity study and the prenatal developmental toxicity study sequentially. In fact, the deadline to submit the required studies is already set to allow sequential testing.

4. Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.) in a first species

Pursuant to Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

A "pre-natal developmental toxicity study" (test method EU B.31./OECD TG 414) for a first species is a standard information requirement as laid down in Annex IX, Section 8.7.2. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

In the technical dossier you have provided a study record for an OECD TG 422 screening study. You have also sought to adapt this information requirement by provided the following justification for the adaptation:
"*Developmental studies in either the rat or the rabbit are not scientifically justified. In an OECD 422 reproduction/developmental screening study with repeat oral dosing for 28-days, lower mean F1 birth weights, pup body weight gains during PND 1-4 and pup body weights on PND 4 were observed at the highest dose level of 1000 mg/kg bw/day in male and female rats. Adverse effects (lower mean food consumption and granulomatous inflammation of the mesenteric lymph node in the males and females) were also noted at 1000 mg/kg bw/day. The NOAEL for both developmental and systemic toxicity was therefore considered to be 500 mg/kg bw/day in the absence of adverse effects at this dose level. In the absence of reproductive/developmental effects at dose levels below those at which maternal systemic toxicity is observed further investigations into the effects of the test material on reproduction parameters are considered to be scientifically unjustified. There is no evidence that boric acid has a mechanism of action relating to endocrine disruption.*"

Furthermore, you have submitted an expert statement ([redacted] 2016) to support your adaptation. The expert statement argues that human exposure to the registered substance is limited. It also describes the expected metabolic pathways for the registered substance, with specific regard to its content of boric acid. In addition, the results of the provided OECD TG 422 screening study with the registered substance are described in detail, and effects of boric acid on fertility and developmental toxicity are summarized. With respect to endocrine disruption, you concluded that *"There is no evidence that boric acid has a mechanism of action relating to endocrine disruption and whilst the exact mechanism has not been fully elucidated there are some proposed mechanisms but these do not involve endocrine disruption."*

While you have not explicitly claimed an adaptation, you have provided information that could be interpreted as an attempt to adapt the information requirement according to Annex XI, Section 1.2., weight of evidence. Hence, ECHA has evaluated your adaptation with respect to this provision.

An adaptation pursuant to Annex XI, Section 1.2. requires sufficient weight of evidence from several independent sources of information leading to the assumption/conclusion that a substance has or has not a particular dangerous property with respect to the information requirement in question including an adequate and reliable documentation.

Your weight of evidence adaptation needs to address the specific dangerous (hazardous) properties of the registered substance at equivalent level as investigated in a pre-natal developmental toxicity study (EU B.31/OECD TG 414). Relevant elements are in particular exposure route, duration and levels, sensitivity and depth of investigations to detect pre-natal developmental toxicity (including growth, survival, external, skeletal and visceral alterations) and maternal toxicity.

You have submitted information from an OECD TG 422 screening study. This study provides limited information on peri- and post-natal toxicity. However, this study does not provide specific information on pre-natal developmental toxicity like skeletal and visceral examinations to investigate the teratogenic potential of a substance. In the expert statement ([redacted] 2016) you summarize studies demonstrating the developmental toxic (including teratogenic) effect of boric acid which has a harmonised classification for reproductive toxicity category 1B (H360FD).
ECHA notes that boric acid is one of the starting materials for manufacturing the registered substance and also a constituent of the registered substance in a concentration range between [redacted] and [redacted]% (w/w). Based on Toolbox predictions, you assume that boric acid is *not* one of the predicted metabolites of the registered substance and you did not classify the registered substance with respect to reproductive toxicity. However, in the absence of specific information of the teratogenic potential of the registered substance, ECHA considers that the provided information is not suitable to allow a conclusion whether the registered substance has pre-natal developmental toxic effects and classification is required or not. Hence, the general rules for adaptation laid down in Annex XI, Section 1.2. of the REACH Regulation are not met and your adaptation of the information requirement is rejected.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to the test method EU B.31./OECD TG 414, the rat is the preferred rodent species and the rabbit the preferred non-rodent species. On the basis of this default assumption ECHA considers testing should be performed with rats or rabbits as a first species.

ECHA considers that the oral route is the most appropriate route of administration for substances except gases to focus on the detection of hazardous properties on reproduction as indicated in ECHA *Guidance on information requirements and chemical safety assessment* (version 6.0, July 2017) R.7a, chapter R.7.6.2.3.2. Since the substance to be tested is a solid, ECHA concludes that testing should be performed by the oral route.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Pre-natal developmental toxicity study (test method: EU B.31./OECD TG 414) in a first species (rat or rabbit) by the oral route.

5. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.)

Pursuant to Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

"Long-term toxicity testing on fish" is a standard information requirement as laid down in Annex IX, Section 9.1.6. of the REACH Regulation. Adequate information on Fish, early-life stage (FELS) toxicity test (Annex IX, 9.1.6.1.), or Fish, short-term toxicity test on embryo and sac-fry stages (Annex IX, 9.1.6.2.), or Fish, juvenile growth test (Annex IX, 9.1.6.3.) needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex IX, Section 9.1.6., column 2. You provided the following justification for the adaptation "*According to REACH Annex IX Section 9.1 Long-term testing will only be proposed if the CSR indicates the need to investigate further effects on aquatic organisms. It is not classified as PBT or vPvB. The CSR did not trigger any concern for long-term exposure. In addition a long-term study on aquatic invertebrates is available with a 21-day NOELR of 10 mg/L loading rate WAF. Therefore a study is scientifically unjustified.*"

Based on the information provided in your dossier (one overall value of water solubility ≤ 0.17 mg/l for the registered UVCB-substance), ECHA considers that some constituents of the registered substance are likely to be poorly soluble.

Poorly soluble substances require longer time to be significantly taken up by the test organisms and so steady state conditions are likely not to be reached within the duration of a short-term toxicity test. For this reason, short-term tests may not give a true measure of toxicity for poorly soluble substances and toxicity may actually not even occur at the water solubility limit of the substance when the test duration is too short. Annex VIII 9.1.3. and Annex VII 9.1.1. of the REACH Regulation explicitly recommend that long-term aquatic toxicity tests are considered if the substance is poorly water soluble on the respective tonnage levels.

The available information in your chemical safety assessment does not allow to omit long-term testing. Moreover, based on Annex VIII, Section 9.1.3. column 2 and according to ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), Chapter R7b (Section R.7.8.5.3), a long-term study shall be considered if the substance is poorly water soluble, i.e. solubility is below 1 mg/L. Therefore, ECHA considers that the short-term toxicity data alone are not appropriate and information on long-term toxicity in fish is needed for the PNEC derivation.

Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) fish early-life stage (FELS) toxicity test (test method OECD TG 210), fish short-term toxicity test on embryo and sac-fry stages (test method EU C.15. / OECD TG 212) and fish juvenile growth test (test method EU C.14. / OECD TG 215) are the preferred tests to cover the standard information requirement of Annex IX, Section 9.1.6.

However, the FELS toxicity test according to OECD TG 210 is more sensitive than the fish, short-term toxicity test on embryo and sac-fry stages (test method EU C.15 / OECD TG 212), or the fish, juvenile growth test (test method EU C.14. / OECD TG 215), as it covers several life stages of the fish from the newly fertilized egg, through hatch to early stages of growth (see ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), *Chapter R7b, Figure R.7.8-4).*

Moreover, the FELS toxicity test is preferable for examining the potential toxic effects of substances which are expected to cause effects over a longer exposure period, or which require a longer exposure period of time to reach steady state (ECHA *Guidance Chapter R7b,* version 4.0, June 2017). The revised OECD test guideline 210 (adopted on 26 July 2013) is a suitable test method for addressing the information requirements of Annex IX, section 9.1.6.1. of the REACH Regulation.

ECHA notes that Member State Competent Authorities submitted Proposals for Amendment (PfAs) where they considered that the aquatic ITS may be applicable in this case and that further advice on possible alternatives for animal testing should be provided in the decision. Based on the PfA ECHA further clarified why the aquatic ITS is not applicable in this case and updated the note for consideration for possible alternatives for animal testing.

In your comments on the PfAs you state that you have conducted a read across analysis by providing QSAR estimations with OECD QSAR Toolbox (version 3.4) based on five nearest neighbours in the Boron Compounds category with experimental FELS data that predicted a NOEC of 13.4 mg/l.

ECHA notes that the documentation is very limited on the proposed analogue approach and no QMRF or QPRF documents nor any other supporting documentation for the read-across approach have been provided to support the approach. ECHA understands that you meant to read-across from other boron compounds (as defined by US EPA New Chemicals Categories), from the screen-shot of the Toolbox prediction, ECHA understands that following source substances are to be used for the read-across: boric acid, dipotassium tetraborate, sodium metaborate and potassium pentaborate.

However, you have not considered the impact of potential degradation (hydrolysis) in the test system for the read-across (to which chemicals the test organisms are exposed to). You have also not considered the differences in the uptake/bioaccumulation potential between the target and the source chemicals. You did not explain how the structures are linked to the predicted property and how the variations in the property are linked to the differences of the source substances within the boron compounds group. From the documentation submitted, it is apparent there are some considerable differences between the source chemicals and the target, which have not been properly addressed e.g. both the target and the source contain boron but while the constituents of the target are borate esters, all the analogues are in fact borates. Furthermore, no considerations on differences in mechanisms for target and source chemicals have been addressed.

ECHA notes that as only the effect values are provided it is not possible for ECHA to assess the reliability and validity of the long term fish data used in the prediction.

Furthermore, no physicochemical and other toxicity data for the source substances were provided to assess the similarity between the substances. The source substances are much smaller, which will result most likely in different properties between the target and source substances.

Additionally, you refer to a JRC report (EC JRC Report 2016: *Scientific options for avoiding chronic fish testing on the basis of existing data and extrapolation approaches*), stating that often acute to chronic toxicity ratio would be 10. In the description of the US EPA boron compounds category however it is indicated that boron compounds exhibit large acute to chronic ratios (ACR) towards fish (125 as a mean ACR).

Moreover, the results from the long-term tests on aquatic invertebrates show some effects, indicating a possible concern for aquatic toxicity.

Therefore, ECHA concludes that:

- the provided QSAR prediction does not meet the conditions listed in REACH Annex IX, 1.3, as they are not adequate for the purpose of classification and labelling and/or risk assessment and no adequate and reliable documentation of the applied method has been provided and
- the provided read-across approach does not meet the conditions listed in REACH Annex IX, 1.5, as they are not adequate for the purpose of classification and labelling and/or risk assessment, have no adequate and reliable coverage of the key parameters addressed in the corresponding test method referred to in Article 13(3) and no adequate and reliable documentation of the applied method has been provided.

ECHA notes that for the derivation of the $PNEC_{aquatic}$ data on three trophic levels, on aquatic invertebrates, fish and aquatic plants, is required (ECHA Guidance on information requirements and chemical safety assessment, v.4.0, June 2017, Chapter R7b, Section R.7.8.5.3). As the short-term data is not applicable in this case, long-term data on all three trophic levels is needed for the derivation of $PNEC_{aquatic}$ and to perform the chemical safety assessment.

Furthermore, ECHA notes that due to the low water solubility the short-term data cannot serve as a compelling evidence to predict relative differences (or lack of) in species sensitivity required to apply the aquatic ITS (*ECHA Guidance on information requirements and chemical safety assessment*, Chapter R.7b (version 4.0, June 2017), Section R.7.8.5.3.).

Lastly, ECHA notes that REACH requires the registrant to consider a long-term study when the substance is poorly water soluble (e.g. water solubility below 1 mg/L or below the detection limit of the analytical method of the test substance based on *ECHA Guidance on information requirements and chemical safety assessment*, Chapter R.7b (version 4.0, June 2017), Section R.7.8.5.). Therefore, in this case long-term data is required to accurately assess the effects of the low water solubility substance on aquatic organisms.

For the reasons stated above, the aquatic ITS (*ECHA Guidance on information requirements and chemical safety assessment*, Chapter R.7b (version 4.0, June 2017), Section R.7.8.5.3.) is not applicable and it is necessary to provide long-term data on both aquatic invertebrates and on fish.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Fish, early-life stage (FELS) toxicity test (test method: OECD TG 210).

Notes for your consideration

Before conducting the above test under request 5, you are advised to consult the ECHA Guidance on information requirements and chemical safety assessment, Chapters R.4 (v.1.1, December 2011), R.5 (v.2.1, December 2011), R.6 (May 2008), R.7b (v 4.0, June 2017) and R.7c (v 3.0, June 2017). If you decide to adapt the testing requested according to the specific rules outlined in Annexes VI to X and/or according to general rules contained in Annex XI of the REACH Regulation, you are referred to the advice provided in practical guides on "How to use alternatives to animal testing to fulfil your information requirements for REACH registration".

It is important to ensure that the particular sample of substance selected to be tested in the study is appropriate to assess the properties of the registered substance. Hence, it is critical that those constituents which are most relevant should be present at appropriate concentrations in any sample tested. As this relevant information may only become available following environmental fate and behaviour testing, the order of aquatic testing needs to be considered. Moreover, according to Annex XIII, the identification [of PBT and vPvB substances] shall also take account of the PBT/vPvB-properties of relevant constituents of a substance and relevant transformation and/or degradation products. Every impurity present in concentrations at or above 0.1 % (w/w) is deemed to be relevant for the PBT/vPvB assessment.

Therefore, the PBT properties should be assessed for constituents, impurities and additives present in the registered substance in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable.

Due to the low solubility of the substance in water, its high adsorption potential and being a UVCB you should consult OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6 and ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), Chapter R7b, Table R.7.8-3 summarising aquatic toxicity testing of difficult substances for choosing the design of the requested ecotoxicity test(s) and for calculation and expression of the result of the test(s).

6. Simulation testing on ultimate degradation in surface water (Annex IX, Section 9.2.1.2.)

Pursuant to Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

"Simulation testing on ultimate degradation in water" is a standard information requirement as laid down in Annex IX, section 9.2.1.2. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement Annex XI, Section 3.2(a). You provided the following justification for the adaptation : "*In accordance with Annex XI Section 3.2 (a) Information sufficient to derive a PNEC has been provided and a risk assessment for the substance performed. The results of the assessment demonstrate that there is no significant exposure for the identified uses of the substance. Furthermore, the results of the exposure scenario show exposures are below the level of the derived PNECs. Therefore additional testing of the substance is not required.*"

However, ECHA notes that your adaptation does not meet the general rule for adaptation of Annex XI; Section 3.2(a). Annex XI Section 3.2(a) indicates that all conditions (i.e. (i), (ii) and (iii)) need to be fulfilled in order to be able to adapt the information requirement. Annex XI Section 3.2 (a)(i) states that "the results of the exposure assessment covering all relevant exposures throughout the life cycle of the substances demonstrate the abscense of or no significant exposure in all scenarios of the manufacture and all identified uses as referred to in Annex VI Section 3.5". ECHA notes that the registration dossier includes two scenarios where wide dispersive outdoor use of the substance (ERC 8d) is reported (i.e. ES 5 and 7). Taking the provided information into account, the absence of, or "no significant exposure" of the registered substance in all scenarios is not demonstrated.

Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) Aerobic mineralisation in surface water – simulation biodegradation (test method EU C.25. / OECD TG 309) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.2.

One of the purposes of the simulation test is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of the REACH Regulation to decide whether it is persistent in the environment. Annex XIII also indicates that "the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions". The Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-8 (version 3.0 2.1 February 2016) indicates 12°C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment. Performing the test at the temperature of 12°C is within the applicable test conditions of the Test Guideline OECD TG 309. Therefore, the test should be performed at the temperature of 12°C.

In the OECD TG 309 Guideline two test options, the "pelagic test" and the "suspended sediment test", are described. ECHA considers that the pelagic test option should be followed as that is the recommended option for P assessment. The amount of suspended solids in the pelagic test should be representative of the level of suspended solids in EU surface water. The concentration of suspended solids in the surface water sample used should therefore be approximately 15 mg dw/L. Testing natural surface water containing between 10 and 20 mg SPM dw/L is considered acceptable. Furthermore, when reporting the non-extractable residues (NER) in your test results you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you state that "*the OECD 309 is a complicated study especially for a UVCB that is relatively insoluble in water (as is the case with this substance in question). Further, based on Annex IX, the 309 testing does not need to be conducted when the substance is insoluble in water.* [redacted] *instead proposes to run an enhanced ready biodegradation (i.e, enhanced 301 series) test as well as a hydrolysis study (including identification of degradants) instead of the OECD 309 in order to address ECHA?s request for information on ultimate degradation and degradation products. ECHA has previously agreed to the use of enhanced ready biodegradation tests to address P(BT) concerns (e.g,. https://echa.europa.eu/documents/10162/13628/benzoicacid_conclusion_en.pdf).*".

ECHA acknowledges that the testing of this substance may encounter difficulties. However, ECHA also notes that you proposed to perform an enhanced biodegradation test instead of the OECD TG 309. It is unclear why the enhanced biodegradation test would encounter less difficulties to be conducted than the simulation testing on ultimate degradation in surface water.

ECHA notes that the studies on ready and inherent biodegradability contribute information at a screening level whilst simulation tests are adequate to assess degradation kinetics, degradation half-lives, and information about mineralisation and degradation products, such as metabolites and bound residues. ECHA also notes that the substances (and relevant constituents) that degrade in these enhanced biodegradation screening tests must not be considered "readily biodegradable" (unless ready biodegradability without enhancements, *i.e.* in a standard ready biodegradation test, is shown). Furthermore, positive results from enhanced screening tests cannot be used on their own and may only be considered as a part of a weight-of-evidence approach to conclude that a substance is not P/vP. This is reflected in the ECHA Guidance on Information Requirements and Chemical Safety Assessment Chapters R7b and R11.

Since the enhanced ready biodegradation test does not *per se* fulfil the standard information requirement on simulation studies, this study cannot be requested under the dossier evaluation process. The results from the surface water – simulation biodegradation test are thus still needed to fulfil this endpoint.

ECHA further notes that according to Annex XIII of the REACH Regulation, the identification of PBT/vPvB substances shall take account of the PBT/vPvB properties of relevant *constituents* of the substance. Section R.11.4.1 of REACH Guidance document R.11 on PBT/vPvB assessment further indicates that "*constituents, impurities and additives should normally be considered are relevant for the PBT/vPvB assessment when they are present in concentration of ≥ 0.1% (w/w). This limit of 0.1% (w/w) is set based on a well-established practice recognised in European Union legislation*". Therefore, results from the water simulation test (*e.g.* degradation half-lives) shall be identified for each constituent, impurity and additive present in the registered substance in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable.

ECHA notes that Member State Competent Authorities submitted Proposals for Amendment (PfAs) to clarify the testing conditions for surface water simulation test and to request additionally simulation tests on sediment and soil based on the substance properties. Based on the PfA ECHA further clarified the testing requirements for surface water and added requests for soil and sediment simulation testing, sections 7 and 8 below.

In your comments on the PfAs you state that "*The OECD 301B ready biodegradation test is a very stringent method for biodegradation, and the 28 day biodegradation result for this substance was greater than 20% -- thereby indicating that although the substance did not readily biodegrade the substance is inherently degradable. Even though the substance is inherently degradable, as a worst case approach for the CSR the PBT assessment in the dossier already considered the substance Persistent (not vP).* "

ECHA notes that as already stated above the studies on ready and inherent biodegradability contribute information at a screening level whilst simulation tests are adequate to assess degradation kinetics, degradation half-lives, and information about mineralisation and degradation products, such as metabolites and bound residues. Furthermore, negative results from a screening study can only conclude that the substance is potentially P. ECHA notes further that degradation simulation studies are the only tests that can provide a definitive degradation half-life that can be compared directly to the persistence criteria as further discussed in the ECHA Guidance on Information Requirements and Chemical Safety Assessment Chapters R7b and R11 (specifically section R.11.4.1.1.1 Integrated assessment and testing strategy (ITS) for persistence assessment).

Moreover, you have not considered the degradation products exceeding >0.1% (w/w) in your PBT assessment.

You acknowledge in your comments that the substance has low water solubility and high log P, supporting the additional requests for degradation simulation in soil and sediment simulation tests as proposed by the MSCA.

You also state in your comments that biodegradation models for this substance using EPISuite/OECD Toolbox predict a lack of persistency which adds further weight of evidence in support of inherent degradation and a lack of necessity for further testing. However, you have not provided any QMRF or QPRF data to support that statement. Therefore, ECHA concludes that you have not provided enough information to support QSAR prediction and therefore the information does not meet the conditions listed in REACH Annex IX, 1.3.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic mineralisation in surface water – simulation biodegradation test (test method: EU C.25./OECD TG 309);

Notes for your consideration for requests (6) – (8)

Before conducting the requested tests you are advised to consult the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Sections R.7.9.4 and R.7.9.6 (version 4.0, June 2017) and Chapter R.11, Section R.11.4.1.1 (version 3.0, June 2017) on PBT assessment to determine the sequence in which the simulation tests are to be conducted and the necessity to conduct all of them. The order in which the simulation biodegradation tests are performed needs to take into account the intrinsic properties of the registered substance and the identified use and release patterns which could significantly influence the environmental fate of the registered substance.

In accordance with Annex I, Section 4, of the REACH Regulation you should revise the PBT assessment when results of the tests from requests (6) to (8) are available. You are also advised to consult the ECHA Guidance on information requirements and chemical safety assessment (version 3.0, June 2017), Chapter R.11, Section R.11.4.1.1. and Figure R. 11-3 on PBT assessment for the integrated testing strategy for persistency assessment in particular taking into account the degradation products of the registered substance.

7. Soil simulation testing (Annex IX, Section 9.2.1.3.)

"Soil simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.3. of the REACH Regulation for substances with a high potential for adsorption to soil. The registered substance has low water solubility (≤ 0.17 mg/l), high partition coefficient (log Kow 6.24 to > 9.4) and high adsorption coefficient (log Koc,soil >5.63), indicating high adsorptive properties. Therefore, adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex XI, Section 3.2 of the REACH Regulation. You provided the following justification for the adaptation: "*In accordance with Annex XI Section 3.2 (a) Information sufficient to derive a PNEC has been provided and a risk assessment for the substance performed. The results of the assessment demonstrates that there is no significant exposure for the identified uses of the substance. Furthermore, the results of the exposure scenario show exposures are below the level of the derived PNECs. Therefore additional testing of the substance is not required.*"

However, ECHA notes that your adaptation does not meet the general rule for adaptation of Annex XI, Section 3.2. that in all cases, adequate justification and documentation shall be provided and that the justification shall be based on a thorough and rigorous exposure assessment in accordance with section 5 of Annex I. ECHA notes that you have used sector specific environmental release categories (SpERCs) in all the exposure scenarios (ES) without further justification (supported by specific operational conditions and/or risk management measures to reach the SpERC release factor) on the use of the significantly lower release factors compared to the default ERC values. ECHA notes that if ERC values would have been used, RCRs for those compartments would have been above 1, i.e. not demonstrating low exposure of the substance to the environment.

According to the ECHA *Guidance on information requirements and chemical safety assessment* Chapter R.16 (version: 3, February 2016) the exposure scenario should contain information about operational conditions and risk management measures based on which the assumed release factors and daily use rates can be justified. Exposure scenarios making reference to the A and B tables of the Technical Guidance Document (TGD, 2003) without providing more specific information on the conditions of use are considered insufficient to meet the REACH requirements. Furthermore, the Guidance indicates that sector specific environmental release categories (spERCs) developed by industrial sector organisations can be used in place of the conservative default environmental release categories (ERCs) of ECHA guidance. As far as possible, spERCs have to be linked to the applied RMM and OC driving the release estimation.

In the present case, in the CSR you have provided seven ESs: 1) formulation; 2) use at industrial site, GES use group B; 3) use at industrial site, GES use group C; 4) professional use, GES use group B; 5) professional use, GES use group C; 6) consumer use, GES use group B; and 7) consumer use, GES use group C.

ECHA notes that, in order to cover any exposures that may be related to the identified hazards, exposure estimation for all of the ESs as stated by you in the CSR is based on sector specific environmental release category (spERC) release factors.

ECHA considers that an adequate and detailed justification (e.g. based on RMMs and/or OCs and/or substance properties) of release factors used in exposure estimation, other than the default ERC release factors, is not provided in the CSR (e.g. it is not clear whether the reduced release factors from A and B tables are used in exposure estimation or these factors are reduced by efficiencies of RMMs which are noted in the ESs etc.). Where internal measurements of releases are available, the summary of results of these measurements is needed. This summary should be detailed enough to understand whether or not it covers relevant scenarios for possible releases from the substance processing according to the relevant ES.

According to Annex IX, Section 9.2.1.3, column 2 of the REACH Regulation, simulation testing on soil does not need to be conducted if the substance is readily biodegradable or if direct or indirect exposure of soil is unlikely. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable in 28 days (26.7% CO2 evolution according to OECD TG 301B. Regarding the exposure to soil, the substance has a low water solubility (≤ 0.17 mg/l), high partition coefficient (log Kow 6.24 to > 9.4) and high adsorption coefficient (log Koc,soil >5.63), indicating high adsorptive properties. Furthermore, based on the uses reported in the technical dossier, ECHA considers that such uses are reported for which soil exposure cannot be excluded (e.g. Environmental Release Category (ERC) 8d). ECHA therefore considers that you have not demonstrated that soil exposure is unlikely. Moreover, you have not demonstrated that there is no significant environmental exposure for all the identified uses of the substance as required by Annex XI, Section 3.2 of the REACH Regulation.

ECHA notes also that you have not provided any adequate justification in your chemical safety assessment (CSA) or in the technical dossier for why there is no need to investigate further the degradation of the substance and its degradation products. As explained further below, ECHA considers that the information is needed for the PBT/vPvB assessment and for the identification of the degradation products in relation to the PBT/vPvB assessment.

Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 3.0, February 2016) Aerobic and anaerobic transformation in soil (test method EU C.23. / OECD TG 307) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.3.

One of the purposes of the simulation test is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of REACH Regulation to decide whether it is persistent in the environment. Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-8 (version 3.0 February 2016) indicates 12°C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment. Performing the test at the temperature of 12°C is within the applicable test conditions of the Test Guideline OECD TG 307.

Simulation tests performed in sediment or in soil possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product unless they are irreversibly bound or incorporated into the biomass. When reporting the non-extractable residues (NER) in your test results you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic and anaerobic transformation in soil (test method: EU C.23./OECD TG 307). The biodegradation of each relevant constituent present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable shall be assessed. This can be done simultaneously during the same study.

8. Sediment simulation testing (Annex IX, Section 9.2.1.4.)

"Sediment simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.4. of the REACH Regulation for substances with a high potential for adsorption to sediment. The registered substance has low water solubility (≤ 0.17 mg/l), high partition coefficient (log Kow 6.24 to > 9.4) and high adsorption coefficient (log Koc,soil >5.63), indicating high adsorptive properties. Therefore, adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex XI, Section 3.2 of the REACH Regulation. You provided the following justification for the adaptation: "*In accordance with Annex XI Section 3.2 (a) Information sufficient to derive a PNEC has been provided and a risk assessment for the substance performed. The results of the assessment demonstrates that there is no significant exposure for the identified uses of the substance. Furthermore, the results of the exposure scenario show exposures are below the level of the derived PNECs. Therefore additional testing of the substance is not required.*"

However, ECHA notes that your adaptation does not meet the general rule for adaptation of Annex XI; Section 3.2. that in all cases, adequate justification and documentation shall be provided and that the justification shall be based on a thorough and riorous exposure assessment in accordance with section 5 of Annex I. ECHA notes that you have used the SpERCs in all the exposure scenarios without further justification (supported by specific operational conditions and/or risk management measures to reach the SpERC release factor) on the use of the significantly lowere release factors compared to default ERC values. ECHA notes that if ERC values would have been used, RCR's for those compartments would have been above 1, i.e. not demonstrating low exposure of the substance to the environment.

According to the ECHA *Guidance on information requirements and chemical safety assessment* Chapter R.16 (version: 3, February 2016) the exposure scenario should contain information about operational conditions and risk management measures based on which the assumed release factors and daily use rates can be justified. Exposure scenarios making reference to the A and B tables of the Technical Guidance Document (TGD, 2003) without providing more specific information on the conditions of use are considered insufficient to meet the REACH requirements.

Furthermore, the Guidance indicates that sector specific environmental release categories (spERCs) developed by industrial sector organisations can be used in place of the conservative default environmental release categories (ERCs) of ECHA guidance. As far as possible, spERCs have to be linked to the applied RMM and OC driving the release estimation.

In the present case, in the CSR you have provided 7 ESs: 1) formulation; 2) use at industrial site, GES use group B; 3) use at industrial site, GES use group C; 4) professional use, GES use group B; 5) professional use, GES use group C; 6) consumer use, GES use group B and 7) consumer use, GES use group C.

ECHA notes that, in order to cover any exposures that may be related to the identified hazards, exposure estimation for all of the ESs as stated by you in the CSR is based on sector specific environmental release category (spERC) release factors.

ECHA considers that an adequate and detailed justification (e.g. based on RMMs and/or OCs and/or substance properties) of release factors used in exposure estimation, other than the default ERC release factors, is not provided in the CSR (e.g. it is not clear whether reduced release factors from A and B tables are used in exposure estimation or these factors are reduced by efficiencies of RMMs which are noted in the ESs etc.). Where internal measurements of releases are available, the summary of results of these measurements is needed. This summary should be detailed enough to understand whether or not it covers relevant scenarios for possible releases from the substance processing according to the relevant ES.

According to Annex IX, Section 9.2.1.3, column 2 of the REACH Regulation, simulation testing on soil does not need to be conducted if the substance is readily biodegradable or if direct or indirect exposure of soil is unlikely. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable in 28 days (26.7% CO2 evolution according to OECD TG 301B. Regarding the exposure to sediment, the substance has a low water solubility (≤ 0.17 mg/l), high partition coefficient (log Kow 6.24 to > 9.4) and high adsorption coefficient (log Koc,soil >5.63), indicating high adsorptive properties. Furthermore, based on the uses reported in the technical dossier, ECHA considers that such uses are reported for which sediment exposure cannot be excluded (e.g. Environmental Release Category (ERC) 8d). ECHA therefore considers that you have not demonstrated that sediment exposure is unlikely. Moreover, you have not demonstrated that there is no significant environmental exposure for all the identified uses of the substance as required by Annex XI, Section 3.2 of the REACH Regulation.

ECHA notes also that you have not provided any adequate justification in your chemical safety assessment (CSA) or in the technical dossier for why there is no need to investigate further the degradation of the substance and its degradation products. As explained further below, ECHA considers that the information is needed for the PBT/vPvB assessment and for the identification of the degradation products in relation to the PBT/vPvB assessment.

Therefore, your adaptation of the information requirement cannot be accepted.

As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 3.0, February 2016) Aerobic and anaerobic transformation in soil (test method EU C.23. / OECD TG 307) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.3.

One of the purposes of the simulation test is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of REACH Regulation to decide whether it is persistent in the environment. Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-8 (version 3.0 February 2016) indicates 12°C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment. Performing the test at the temperature of 12°C is within the applicable test conditions of the Test Guideline OECD TG 308.

Simulation tests performed in sediment or in soil possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product unless they are irreversibly bound or incorporated into the biomass. When reporting the non-extractable residues (NER) in your test results you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic and anaerobic transformation in aquatic sediment systems (test method: EU C.24./OECD TG 308). The biodegradation of each relevant constituent present in concentration at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable shall be assessed. This can be done simultaneously during the same study.

9. Identification of degradation products (Annex IX, 9.2.3.)

Pursuant to Articles 10(a) and 12(1) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation. The information to be generated for the dossier must fulfil the criteria in Article 13(4) of the same regulation.

The identification of the degradation products is a standard information requirement according to column 1, Section 9.2.3. of Annex IX of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

The technical dossier does not contain information or an adaptation in accordance with column 2 of Annex IX, Sections 9.2 or 9.2.3. or with the general rules of Annex XI for this standard information requirement.

According to Annex IX, Section 9.2.3., column 2 of the REACH Regulation, identification of degradation products is not needed if the substance is readily biodegradable. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable.

Furthermore, ECHA notes that you have not provided any justification in your chemical safety assessment (CSA) or in the technical dossier for why there is no need to provide information on the degradation products.

Pursuant to Annex XIII of the REACH Regulation "*the identification* [of PBT and vPvB substances] *shall also take account of the PBT/vPvB-properties of relevant constituents of a substance and relevant transformation and/or degradation products*". ECHA Guidance on information requirements and chemical safety assessment (version 3.0, June 2017), Chapter R.11.4.1. further specifies that "*constituents, impurities and additives are relevant for the PBT/vPvB assessment when they are present in concentration of ≥ 0.1% (w/w). This limit of 0.1% (w/w) is set based on a well-established practice rooted in a principle recognised in European Union legislation*. [...] *Similar arguments apply to relevant transformation/degradation products. The PBT/vPvB assessment should normally be carried out for each relevant transformation or degradation product*". ECHA notes that your CSA does not contain any information on whether the degradation products could be PBT/vPvB or not.

Information on degradation products shall also be taken into account for the exposure assessment (Annex I 5.2.4. of the REACH Regulation) and for the hazard assessment (e.g. column 2 of Annex X 9.4 and Annex X 9.5.1 of the REACH Regulation). Finally, information on degradation products is required for the preparation of Section 12 of the safety datasheet (Annex II of the REACH Regulation).
As explained above, the information provided on this endpoint for the registered substance in the technical dossier does not meet the information requirements. Consequently there is an information gap and it is necessary to provide information for this endpoint.

Aerobic mineralisation in surface water – simulation biodegradation (test method EU C.25. / OECD TG 309) is an appropriate test to obtain information on the primary degradation and the formation of major transformation products for substances that are not highly insoluble in water. Based on the information provided in your registration dossier, ECHA notes that the water solubility of the substance is ≤0.17 mg/L, therefore the registered substance cannot be regarded as highly insoluble in water. The analytical methods to be applied will have to be substance-specific in order to identify the transformation products. When analytically possible, the identification, stability, behaviour and molar quantity of those transformation products relative to the parent compound should be evaluated. In addition, degradation half-life, log Kow and potential toxicity of the transformation products may be investigated. As specified in the OECD 309 test guideline, higher concentrations of the test substance (e.g., >100 µg/L) could be used for the identification and quantification of major transformation products to overcome potential analytical limitations.

In your comments to the draft decision you state that "*the OECD 309 is a complicated study especially for a UVCB that is relatively insoluble in water (as is the case with this substance in question). Further, based on Annex IX, the 309 testing does not need to be conducted when the substance is insoluble in water.* [redacted] *instead proposes to run an enhanced ready biodegradation (i.e, enhanced 301 series) test as well as a hydrolysis study (including identification of degradants) instead of the OECD 309 in order to address ECHA?s request for information on ultimate degradation and degradation products. ECHA has previously agreed to the use of enhanced ready biodegradation tests to address P(BT) concerns (e.g,. https://echa.europa.eu/documents/10162/13628/benzoicacid_conclusion_en.pdf).*".

ECHA notes that, while studies on ready and inherent biodegradability contribute with information at a screening level, simulation tests are adequate to assess degradation kinetics, degradation half-lives, and information about mineralisation and degradation products (metabolites, bound residues). In addition, since the enhanced ready biodegradation test does not *per se* fulfil the standard information requirement on identification of degradation products, this study cannot be requested under dossier evaluation process, and therefore the results from the surface water – simulation biodegradation test are still needed to fulfil this endpoint.

Thus, the required to identify the degradation products is a simulation test. However, if each relevant constituent of the substance fulfils the readily biodegradability criteria, this endpoint can be adapted based on column 2 of the Annex IX, Section 9.2.3..

ECHA would like to remind you that according to Annex XIII of the REACH Regulation, the identification of PBT/vPvB substances shall take account of the PBT/vPvB-properties of relevant constituents of the substance. Therefore the degradation products shall be identified for each constituents, impurities and additives present in the registered substance in concentrations at or above 0.1% (w/w) or, if not technically feasible, in concentrations as low as technically detectable.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Identification of the degradation products (Annex IX, Section 9.2.3.) using one of the tests mentioned in sections 6-8 above. The degradation product of each constituent and impurity present in concentrations at or above 0.1% (w/w) shall be identified.

10. PBT and vPvB assessment (Annex I, Section 4.)

Pursuant to Articles 10(b) and 14(1) of the REACH Regulation the registration shall contain a chemical safety report (CSR) which shall document the chemical safety assessment (CSA) conducted in accordance with Article 14(2) to (7) and with Annex I of the REACH Regulation.

Pursuant to Sections 0.6.1. and 4 of Annex I of the REACH Regulation a chemical safety assessment (CSA) performed by a Registrant shall include the PBT and vPvB assessment. Section 4.0.1. of Annex I notes that the objective of the PBT and vPvB assessment shall be to determine if the substance fulfils the criteria given in Annex XIII and if so, to characterise the potential emissions of the substance. Annex XIII of the REACH Regulation lays down the criteria for the identification of persistent, bioaccumulative and toxic substances (PBT substances), and very persistent and very bioaccumulative substances (vPvB substances) as well as the information that must be considered for the purpose of assessing the P, B, and T properties of a substance.

Pursuant to the fifth introductory paragraph of Annex XIII, the identification of PBT/vPvB substances shall also take account of the PBT/vPvB-properties of relevant constituents of a substance and of relevant degradation products. Every impurity present in concentrations at or above 0.1 % (w/w) is deemed to be relevant for the PBT/vPvB assessment.

ECHA notes that you have summarised the outcome of the PBT and vPvB assessment of the substance in the CSR attached to the technical dossier as well as in Section 2.3 of IUCLID. You have concluded that the substance is considered to be persistent (P) but not bioaccumulative (not B) nor toxic (not T), and therefore that the substance is not PBT/vPvB.

You have sought to justify the non-B property of the registered substance with: "*The experimentally derived Log Pow value for the substance has been identified as > 9.4. QSAR calculations of Log Pow for the components determined that Log Pow >10 for the majority of the components. ECHA Guidance on Information requirements and chemical safety assessment Chapter R11: PBT assessment on determination of bioaccumulation potential states: The aquatic BCF of a substance is probably lower than 2000 L/kg if the calculated log Pow is higher than 10.*"

ECHA notes that a measured Log Pow range from 6.24 to > 9.4 has been provided but that the chemical safety report and the technical dossier do not include results nor calculations of Log Pow for the individual constituents or groups of homogeneous constituents. ECHA acknowledges that constituents with very high Log Kow are unlikely to be bioaccumulated because of their limited bioavailability from water. However, for the constituents (or groups of homogeneous constituents) which have lower log Kow values, ECHA considers that is it not possible to rule out that they could bioaccumulate.

Furthermore, ECHA notes that you have registered the substance as composed of 9 constituents, and you have provided 3 QSAR values to prove the low BCF of the substance. Annex XI Section 1.3 establishes that results of (Q)SARs may be used instead of testing when the following conditions are met:

- results are derived from a (Q)SAR model whose scientific validity has been established,
- the substance falls within the applicability domain of the (Q)SAR model,
- results are adequate for the purpose of classification and labelling and/or risk assessment, and
- adequate and reliable documentation of the applied method is provided.

ECHA notes that you have failed to identify the constituents to which belong the reported BCF, to include a reasoning on why you provide QSAR results for those 3 specific constituents and to provide documentation on the QSAR that would include justification on whether the constituents are within the applicability domain of the used model.

There is also no indication in the CSR or in the technical dossier that PBT/vPvB properties of any relevant degradation products were considered in the PBT and vPvB assessment. The information on degradation products of the registered substance is incomplete (see Appendix I, 7. above). ECHA concludes that the consideration of degradation products of the registered substance in the PBT and vPvB assessment is missing.

In the present decision, you have been requested to provide information from the OECD TGs 307, 308, 309 and 210 (Appendix 1, Sections 5-8 above). Once you have obtained the results from these studies (DT50 and NOEC), you can use them to update the P and T properties of the registered substance.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to revise the PBT and vPvB assessment including PBT and vPvB assessment for the relevant constituents of the substance (including all impurities present in concentrations at or above 0.1 % (w/w)) and for the relevant degradation products.

Deadline to submit the requested information in this decision

In the draft decision communicated to you, the time line to provide the requested studies and submit the study results to ECHA in a dossier update was 24 months from the date of adoption of the decision. In your comments on the draft decision, you requested an extension of this timeline to 36 months to allow for sequential testing. You justified this request by providing a letter from a testing laboratory that confirms that 36 months is required for the tests requested in this decision.

Based on the provided information, ECHA agrees to prolong the deadline with 12 months. Hence, the timeline to submit the requested information in an updated registration dossier has been extended from 24 months to 36 months.

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

The compliance check was initiated on 11 November 2016.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA took into account your comments and did not amend the requests. However, the deadline was amended.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

ECHA received proposal(s) for amendment and modified the draft decision.

ECHA invited you to comment on the proposed amendment(s).

ECHA referred the draft decision to the Member State Committee.

Your comments on the proposed amendment(s) were taken into account by the Member State Committee.

The Member State Committee reached a unanimous agreement on the draft decision in its MSC-55 written procedure and ECHA took the decision according to Article 51(6) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

1. This compliance check decision does not prevent ECHA from initiating further compliance checks on the present registration at a later stage.

2. Failure to comply with the request(s) in this decision, or to fulfil otherwise the information requirement(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.

3. In relation to the information required by the present decision, the sample of the substance used for the new tests must be suitable for use by all the joint registrants. Hence, the sample should have a composition that is suitable to fulfil the information requirement for the range of substance compositions manufactured or imported by the joint registrants.

It is the responsibility of all joint registrants who manufacture or import the same substance to agree on the appropriate composition of the test material and to document the necessary information on their substance composition. In addition, it is important to ensure that the particular sample of the substance tested in the new tests is appropriate to assess the properties of the registered substance, taking into account any variation in the composition of the technical grade of the substance as actually manufactured or imported by each registrant.

If the registration of the substance by any registrant covers different grades, the sample used for the new tests must be suitable to assess these grades. Finally there must be adequate information on substance identity for the sample tested and the grades registered to enable the relevance of the tests to be assessed.