ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 24 July 2019

Addressee: [redacted]

Decision number: CCH-D-2114476254-46-01/F
Substance name: Cyclohexylidenebis[tert-butyl] peroxide
EC number: 221-111-2
CAS number: 3006-86-8
Registration number: [redacted]
Submission number: [redacted]
Submission date: 10/05/2016
Registered tonnage band: 100-1000

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

2. **Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.; test method: Daphnia magna reproduction test, EU C.20./OECD TG 211) with the registered substance;**

3. **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;**

4. **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) at a temperature of 12 °C with the registered substance;**

5. **Soil simulation testing (Annex IX, Section 9.2.1.3.; test method: Aerobic and anaerobic transformation in soil, EU C.23./OECD TG 307) at a temperature of 12 °C with the registered substance;**

6. **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) at a temperature of 12 °C with the registered substance;**

7. **Identification of degradation products (Annex IX, Section 9.2.3.)**

8. **Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD TG 305,**

aqueous exposure or dietary exposure) with the registered substance;

9. **Identification of PNEC and risk characterisation (Annex I, Section 3.3.1. and 6.): revise PNECs for freshwater, marine water, freshwater sediment, marine sediment and soil using the assessment factors recommended by ECHA and revise the risk characterisation accordingly *or* provide a detailed justification for not using the recommendations of ECHA guidance in PNEC derivation.**

You have to submit the requested information in an updated registration dossier by **1 August 2022**. You also have to 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 and 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, has to 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 **Ofelia Bercaru**, Head of Unit, Hazard Assessment

[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

TOXICOLOGICAL AND ECOTOXICOLOGICAL INFORMATION

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

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

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.

You have provided a study record for a screening study according to OECD 422 with the registered substance. However, this study does not provide the information required by Annex IX, Section 8.7.2., because it does not cover key parameters of a pre-natal developmental toxicity study like examinations of foetuses for skeletal and visceral alterations.

You have sought to adapt the information requirement for a pre-natal developmental toxicity study according to Annex XI, Section 1.5. of the REACH Regulation by providing a study record for a *"prenatal developmental toxicity study"* (according to OECD TG 414) with the analogue substance 1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (CAS 6731-36-8; EC 229-782-3).

According to Annex XI, Section 1.5., two conditions shall be necessarily fulfilled. Firstly, there needs to be structural similarity between substances which results in a likelihood that the substances have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category. Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group (read-across approach). ECHA considers that the generation of information by such alternative means should offer equivalence to prescribed tests or test methods.

Based on the above, a read-across hypothesis needs to be provided. This hypothesis establishes why a prediction for a toxicological or ecotoxicological property is reliable and should be based on recognition of the structural similarities and differences between the source and registered substances[2]. This hypothesis explains why the differences in the chemical structures should not influence the toxicological/ ecotoxicological properties or should do so in a regular pattern. The read-across approach must be justified scientifically and documented thoroughly, also taking into account the differences in the chemical structures. There may be several lines of supporting evidence used to justify the read-across hypothesis, with the aim of strengthening the case.

[2] Please see for further information ECHA *Guidance on information requirements and chemical safety assessment* (version 1, May 2008), Chapter R.6: QSARs and grouping of chemicals.

Due to the different nature of each endpoint and consequent difference in scientific considerations (e.g. key parameters, biological targets), a read-across must be specific to the endpoint or property under consideration. Key physicochemical properties may determine the fate of a compound, its partitioning into a specific phase or compartment and largely influence the availability of compounds to organisms, e.g. in bioaccumulation and toxicity tests. Similarly, biotic and abiotic degradation may alter the fate and bioavailability of compounds as well as be themselves hazardous, bioaccumulative and/or persistent. Thus, physicochemical and degradation properties influence the human health and environmental properties of a substance and should be considered in read-across assessments. However, the information on physicochemical and degradation properties is only a part of the read-across hypothesis, and it is necessary to provide additional justification which is specific to the endpoint or property under consideration.

The ECHA Read-across assessment framework foresees that there are two options which may form the basis of the read-across hypothesis[3]- (1) (Bio)transformation to common compound(s)- the read-across hypothesis is that different substances give rise to (the same) common compounds to which the organism is exposed and (2) Different compounds have the same type of effect(s)- the read-across hypothesis is that the organism is exposed to different compounds which have similar (eco)toxicological and fate properties as a result of structural similarity (and not as a result of exposure to common compounds).

Finally, Annex XI, Section 1.5. lists several additional requirements, which deal with the quality of the studies which are to be read-across.

You consider to achieve compliance with the REACH information requirement for a pre-natal developmental toxicity study for the registered substance 1,1-bis(tert-butylperoxy)cyclohexane (EC No. 221-111-2) (the 'target substance') using data of a structurally similar substance 1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (EC No 229-782-3) (hereafter the 'source substance').

You have provided a read-across documentation as a separate attachment including QSAR toolbox profiler reports for the target and source substances.

You use the following arguments to support the prediction of properties of the registered substance from data from the source substance:

"Adequate, reliable and available scientific information indicates that the source and target substance have similar toxicological profiles and that data for the source substance are reliable to predict the toxicity of the source substance. These information are further confirmed by applying the OECD QSAR toolbox."

"read-across is based on the hypothesis that source and target substances have the same type of toxicological effects based on common underlying mechanisms"
"systemic toxicity is not relevant for the read-across endpoint developmental toxicity."

"it is anticipated that the target substance shows the same developmental toxicity as the source substance."

As an integral part of this prediction, you propose that the source and registered

[3] Please see ECHA's Read-Across Assessment Framework (https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across).

substance(s) have similar properties for the above-mentioned information requirements. ECHA considers that this information is your read-across hypothesis.

ECHA's evaluation and conclusion

Your proposed adaptation argument is that the similarity in chemical structure and in some of the physico-chemical, toxicological properties between the source and registered substance is a sufficient basis for predicting the properties of the registered substance for other endpoints. Structural similarity is a prerequisite for applying the grouping and read-across approach. However similarity in chemical structure and similarity of some of the physico-chemical and toxicological properties does not necessarily lead to predictable or similar human health properties in other endpoints. Your justification has not established why the prediction is reliable for the developmental toxicity endpoint which is addressed in this decision. More specifically, ECHA notes that the provided prenatal developmental toxicity study (OECD TG 414), with the source substance, and the screening study (OECD TG 422), with the target substance, did not report any reproductive or developmental toxic findings. However, the dosing applied in the screening study with the target substance (high dose group 600 mg/kg bw/day) did not go up to the limit dose, and was therefore considerably lower than in the prenatal developmental toxicity study with the source substance which applied doses up to the limit dose.

Moreover, ECHA notes that the reported test item purity for the screening study and the prenatal developmental toxicity study is 78.6% and 93.4 % with the target and source substances, respectively. ECHA therefore considers, due to dilution of the target substance test item, that the applied dosing further led to a decrease of the dosing with the target substance.

ECHA acknowledges the OECD QSAR toolbox predictions for the target and source substances stating that there is "*not known precedent reproductive and developmental toxic potential.*" However, ECHA notes that in the absence of further data and documentation of the studies used as a basis for the prediction, this statement on its own is not sufficient to support your read-across adaptation.

In your comments to the draft decision, you clarify the QSAR Toolbox profiler output is not intended as standalone information. In addition, you clarify that the highest dose tested in the OECD TG 422 study with the registered substance "*induced clear signs of toxicity, but no unnecessary suffering of the animals. Thus, dose setting is in well accordance with the respective guideline. Therefore, the highest dose level can be by no means considered as too low.*" You note that "*in the OECD 422 study with the target substance all parameters that could indicate developmental impairment were unremarkable, even at the highest dose level inducing systemic toxicity in the parental animals.*"

Furthermore, you provided a revised read-across justification as Annex I to your comments on the draft decision. Within this Annex, and in the actual comments to the draft decision, you referred to a 52 and a 13-week study with the source substance for which you indicated a NOAEL of 20 mg/kg bw/d. By correcting for the content of "active ingredient" (a.i.), you concluded on a NOAEL of 19.8 mg a.i./kg bw/d for the source substance, and based on the screening study (OECD TG 422) provided in the dossier, 118.5 mg a.i./kg bw/d for the target substance. You conclude that the the source substance is a worst case for the target substance with respect to repeated toxicity. With respect to effects on reproduction, you conclude that the source substance did not induce pre-natal developmental toxic effects when tested up to the limit dose, and that "*in the OECD 422 study with the target*

substance all parameters that could indicate developmental impairment were unremarkable, even at the highest dose level inducing systemic toxicity in the parental animals."

ECHA acknowledges these clarifications and notes that they should be included in your read-across supporting documentation in the dossier, as the submission subject to this decision ([redacted]) does not contain these clarifications. ECHA will then accept your read-across adaptation supported by the updated read-across supporting documentation after deadline of this decision. Hence, the request of a pre-natal developmental toxicity study with the registered substance will remain in the decisision for procedural reasons, as the read-across approach does not currently comply with the general rules of adaptation as set out in Annex XI, Section 1.5. of the REACH Regulation.

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

Therefore, the information provided on this endpoint for the registered substance in the technical dossier does not currently 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 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) Chapter R.7a, Section R.7.6.2.3.2. Since the substance to be tested is a liquid, 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: OECD TG 414) in a first species (rat or rabbit) by the oral route.

2. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.)

"Long-term toxicity testing on aquatic invertebrates" is a standard information requirement as laid down in Annex IX, Section 9.1.5. 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 not provided any study record of a long-term toxicity on aquatic invertebrates in the dossier that would meet the information requirement of Annex IX, Section 9.1.5.

You have sought to adapt this information requirement according to Annex IX, Section 9.1.5., column 2. You provided the following justification for the adaptation : "*REACH Regulation (EC) No 1907/2006, Annex IX, Sect. 9.1, Col. 2, states as follows: "9.1.: Long-term toxicity testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the effects on aquatic organisms. The choice of the appropriate tests(s) depends on the results of the chemical safety assessment." A study assessing the long-term toxicity of the test item cyclohexylidenebis[tert-butyl] peroxide towards aquatic invertebrates (Daphnia sp.)*

according to OECD 211 guideline is currently not available. The studies assessing the short-term toxicity of the test item towards fish, aquatic invertebrates (Daphnia sp.) and alage clearly show no adverse effects up to the test item's water solubility. In order to support this finding, a study assessing the long-term toxicity towards aquatic invertebrates (Daphnia sp.) according to OECD 211 guideline will be conducted, since the risk assesment (see PNEC derivation in IUCLID section 6) indicates the nedd to investigate further the effects on aquatic organisms. The study assessing the long-term toxicity of the test item towards aquatic invertebrates (Daphnia sp.) will be ordered. As soon as the study report is available the dossier and the Chemical Safety Report (CSR) will be upadated accordingly. "

However, ECHA notes that your adaptation does not meet the specific rules for adaptation of Annex IX, Section 9.1.5., column 2 because the study is still not made available in the IUCLID dossier.

Moreover, ECHA considers that substances that are poorly soluble in water 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 such substances and toxicity may actually not even occur at the water solubility limit of the substance if the test duration is too short.

ECHA notes that the registered substance is poorly water soluble (WS < 1mg/l, aprox 0.6 mg/l) and hence, information provided on short-term toxicity to aquatic invertebrates showing no effects up to the water solubility limit is not considered reliable as the substance is poorly water soluble.

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

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you agree to perform the test as requested.

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) *Daphnia magna* reproduction test (test method EU C.20. / OECD TG 211) is the preferred test to cover the standard information requirement of Annex IX, Section 9.1.5.

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: Daphnia magna reproduction test (test method: EU C.20./OECD TG 211).

Notes for your consideration

Once results of the test on long-term toxicity to aquatic invertebrates are available, you shall revise the chemical safety assessment as necessary according to Annex I of the REACH Regulation.

Due to the low solubility of the substance in water and hydrolytic properties, you should consult OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6/REV1 (6 July 2018) 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).

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

"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 not provided any study record of a long-term toxicity on fish in the dossier that would meet the information requirement of Annex IX, Section 9.1.6.1 / 9.1.6.2 / 9.1.6.3.

You have sought to adapt this information requirement according to Annex VIII, Section 9.1.3., column 2, with the following justification.
"The performance of a test for long-term toxicity to fish was considered scientifically not justified. REACH Regulation (EC) No 1907/2006, Annex VIII, Sect. 9.1.3, Col. 2, states as follows: "9.1.3: The study (long-term toxicity to fish) does not need to be conducted if: - there are mitigating factors indicating that aquatic toxicity is unlikely to occur, for instance if the substance is highly insoluble in water or the substance is unlikely to cross biological membranes" The test item is not stable in aquatic environment. Due to the unstable nature of organic peroxides, it can be assumed that upon contact with water and organic matter, the test item undergoes rapid degradation resulting in the formation of respective alcohols and acids. In addition, the substance is poorly water soluble and has a adsorption coefficient (log Koc) < 3 (log Koc = 2.69). Thus, the CSR does not show a need for an additional long-term aquatic test. Risk assessment is based on the short-term tests for all throphic levels."
ECHA points out that this adaptation possibility refers to the standard information requirement on short-term toxicity testing on fish.

ECHA also notes that your adaptation does not meet the specific rules for adaptation of Annex IX, Section 9.1.6., column 2 as explained further below.

Moreover, ECHA considers that substances that are poorly soluble in water 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 such substances and toxicity may actually not even occur at the water solubility limit of the substance if the test duration is too short.

ECHA notes that the registered substance is poorly water soluble (WS < 1mg/l, aprox 0.6 mg/l).

Moreover, ECHA notes that the substance is not readily biodegradable (degradation in OECD 301B test 5% in 28d) and the hydrolysis is not rapid but moderate or slow following the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6. ECHA notes that you concluded in IUCLID dossier that the half-life at pH = 4, 7 and 9 at 20 °C are 40 hours, 80 hours and 109 hours, respectively. The value

used for chemical safety assessment is DT50 = 127 hours at 12 °C, pH 4. Hence, ECHA concludes that the substance is not unstable in the aquatic environment.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you consider that the test is not needed for the following reasons:

-the long-term toxicity study on aquatic invertebrates will be conducted and you consider that this study will cover the chemical safety assessment for the aquatic compartment.

-no exposure of the substance is expected to the aquatic compartment based on the substance's use profile and the formation of non-extractable residues.

-the substance will not be persistent in the aquatic compartment;

-in case of environmental exposure, the substance is expected to be of more concern for terrestrial and sediment compartment.

-you plan to cover this endpoint with the data on analogue substance (1,1-bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane. CAS 6731-36-8) for sediment and terrestrial toxicity;

-the substance is an organic peroxide covered by the REACH Organic Peroxide Consortium and that based on the very big dataset available for more than 30 organic peroxides, algae were found to be the most sensitive species for the majority of the substances;

-animal welfare reasons, as a a vertebrate study is always the last resort as stated in REACH Article 25. You use this to support the application of an integrated testing strategy.

In response, ECHA has the following observations.

First, as already explained, for this kind of substance (poorly water soluble with no effects in short-term studies) long-term toxicity data is necessary both on daphnia and fish.

Second, your claim that no exposure of the aquatic compartment is expected due to the covalently bound non-extractable residue, is not supported by further substance specific data and the IUCLID file attached to your comments notes that the substance only probably forms NERs.

Third, based on the data available in the dossier, the substance is not readily biodegradable, is poorly water soluble (not highly insoluble) and potentially highly adsorptive, indicating that all the compartments (water, sediment and soil) are relevant for this kind of substance. In the exposure scenarios as presented in the chemical safety report there were several risk characterisation ratios (RCR's) close to 1 (for water, sediment and soil compartments) for several exposure scenarios e.g. exposure scenarios 4 and 5, indicating that the exposure cannot be considered to be non-existent for any of these compartments.

Fourth, as the requested long-term study on daphnia and the proposed new exposure assessment are not yet available in the dossier, ECHA cannot evaluate the information and make conclusions on the approach proposed. Therefore, ECHA will assess the approach in the latest dossier update in the follow-up process according to Art 42 of the REACH Regulation whether the provisions of REACH Regulation are met.

Fifth, ECHA has not evaluated the data of the analogue substance on toxicity to soil and sediment organisms as this kind of data cannot be used to adapt the current data requirement under the second column of Annex IX, section 9.1.6.1. and Annex XI of the REACH Regulation.

Sixth, the assumption that algae are the most sensitive species for this substance as well is a speculation that is not supported by further evidence. ECHA notes that this substance is no longer part of tert-butyl peroxides group.

Seventh, ECHA agrees that Article 25 REACH requires registrant to avoid unneccessary animal testing. However, in this case ECHA considers animal testing necessary. Furthermore, as explained in the notes for consideration below, an integrated testing strategy cannot be applied for this kind of substance.

For these reasons ECHA considers that 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) can be performed to cover the standard information requirement of Annex IX, Section 9.1.6.

In your comments to the draft decision, you indicate that should ECHA require the conduct of a study on long-term toxicity in fish, you propose to conduct a juvenile fish growth test (OECD 215) instead of a fish early life stage test (OECD 210). You justify this on the basis that section 9.1.6. first column does not specify any preference which test in section 9.1.6. should be performed and that it should therefore be the responsibility of the Registrant to choose the test design.

In response ECHA notes however that section 9.1.6 does not prevent ECHA from choosing the most adequate test for meeting this information requirement. ECHA further notes that you have not provided any scientific argumentation why the OECD 215 test would be more relevant for this substance than the OECD 210. Indeed ECHA considers that 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, Section R.7.8.4.1.*

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).

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

Once results of the test on long-term toxicity to fish are available, you shall revise the chemical safety assessment as necessary according to Annex I of the REACH Regulation.

ECHA notes that there are no reliable short-term studies available on aquatic invertebrates or on fish for the registered substance.

ECHA notes that due to lack of effects in short-term studies it is not possible to determine the sensitivity of species. Therefore, the Integrated testing strategy (ITS) outlined in ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), Chapter R7b (Section R.7.8.5 including Figure R.7.8-4), is not applicable in this case and the long-term studies on both invertebrates and fish shall be conducted. As the registered substance has a reported low water solubility, long-term studies are indicated.

Due to the low solubility of the substance in water and hydrolytic properties you should consult OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6/REV1 (6 July 2018) 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).

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

"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 not provided any study record of simulation testing of the registered substance on ultimate degradation in water in the dossier.

You have sought to adapt this information requirement according to Annex IX, Section 9.2., column 2. You provided the following justification for the adaptation: *"The performance of simulation tests for biodegradation in water and sediment is scientifically unjustified. REACH Regulation (EC) No 1907/2006, Annex IX, Sect. 9.2.1.4., Col. 2, states as follows: "9.2.1.4: The study need not to be conducted: - if the substance is readily biodegradable, or - if direct and indirect exposure of sediment is unlikely. " Direct and indirect exposure of the test item to water and sediment is highly unlikely. Due to the unstable nature of organic peroxides, it can be assumed that upon contact with water and organic matter, the test item undergoes rapid degradation resulting in the formation of respective alcohols and acids. In addition the low adsorption coeffcient (log Koc) of the test item (log Koc=2.69) indicates a low dwell time of the test item in soil and thus a low exposure. Therefore simulation testing for biodegradation in water and sediment was considered not scientifically justified."*

However, ECHA notes that your adaptation does not meet the specific rules for adaptation of Column 2 of Annex IX, Sections 9.2 and 9.2.1.2. for the reasons stated below.

According to Annex IX, Section 9.2.1.2, column 2 of the REACH Regulation, simulation testing on ultimate degradation in surface water does not need to be conducted if the substance is highly insoluble in water or is readily biodegradable. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable in OECD 301B test (5% degradation in 28d) and has a water solubility of < 1 mg/l (aprox 0.6 mg/l).

ECHA notes also 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 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.

Moreover, ECHA notes that the hydrolysis is not rapid but moderate or slow following the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6. ECHA notes that you concluded in IUCLID dossier that the half-life at pH = 4, 7 and 9 at 20 °C are 40 hours, 80 hours and 109 hours, respectively. The value used for chemical safety assessment is DT50 = 127 hours at 12 °C, pH 4. Hence, ECHA concludes that the substance is not unstable in the aquatic environment.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you disagree to perform the test as requested. You have provided a new study on ready biodegradation (OECD 301D, June 2018) and state that no further biotic degradation testing is necessary as there is no direct or indirect exposure to the water compartment.

ECHA notes that the new study on biodegradation reveals that the substance starts degrading to a larger extent only after 112 days. This does not change the conclusion that the substance is not readily biodegradable as the standard ready biodegradability test runs only for 28 days.

ECHA further notes, that based on the data available in the dossier, the substance is not readily biodegradable, is poorly water soluble (not highly insoluble) and potentially highly adsorptive, indicating that all the compartments (water, sediment and soil) are relevant for this kind of substance.

In the exposure scenarios as presented in the CSR there were several RCR's close to [redacted] (for water, sediment and soil compartments) for several exposure scenarios e.g. exposure scenarios 4 and 5, indicating that the exposure cannot be considered to be non-existent for any of these compartments. Moreover, this endpoint can not be adapted based on the claim that there is "no direct or indirect exposure to the compartment" according to column 2 of this data requirement.

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 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. Quantification of non-extractable residues (NER) is also recommended in surface water simulation degradation studies. Furthermore, when reporting NER in your test results you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER as described in Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) and R.11 (version 3.0, June 2017.
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).

5. 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 < 1 mg/l (aprox 0.6 mg/l) and high partition coefficient (log Kow 7.2), 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 not provided any study record of soil simulation testing of the registered substance in the registration dossier.

You have sought to adapt this information requirement according to Annex IX, Section 9.2., column 2. You provided the following justification for the adaptation *"The performance of simulation tests for biodegradation in water and sediment is scientifically unjustified. REACH Regulation (EC) No 1907/2006, Annex IX, Sect. 9.2.1.4., Col. 2, states as follows: "9.2.1.4: The study need not to be conducted: - if the substance is readily biodegradable, or - if direct and indirect exposure of sediment is unlikely. " Direct and indirect exposure of the test item to water and sediment is highly unlikely. Due to the unstable nature of organic peroxides, it can be assumed that upon contact with water and organic matter, the test item undergoes rapid degradation resulting in the formation of respective alcohols and acids. In addition the low adsorption coeffcient (log Koc) of the test item (log Koc=2.69) indicates a low dwell time of the test item in soil and thus a low exposure. Therefore simulation testing for biodegradation in water and sediment was considered not scientifically justified."*

However, ECHA notes that your adaptation does not meet the specific rules for adaptation of Column 2 of Annex IX, Sections 9.2 and 9.2.1.3. for the reasons stated bleow.

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 OECD 301B test (5% degradation in 28d).

Regarding the exposure to soil, the substance has a low water solubility of < 1 mg/l (aprox 0.6 mg/l) and high partition coefficient log Kow 7.2 indicating 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 as the exposure estimations that you provided in the Chemical Safety Report (CSR) indicate that there is exposure to soil in a number of your exposure scenarios (e.g. ES 1, ES 4, ES 5). ECHA therefore considers that you have not demonstrated that soil exposure is unlikely.

ECHA notes also that you have not provided any justification in your chemical safety assessment (CSA) or in the technical dossier 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.

Moreover, ECHA notes that the hydrolysis is not rapid but moderate or slow following the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6. ECHA notes that you concluded in IUCLID dossier that the half-life at pH = 4, 7 and 9 at 20 °C are 40 hours, 80 hours and 109 hours, respectively. The value used for chemical safety assessment is DT50 = 127 hours at 12 °C, pH 4. Hence, ECHA concludes that the substance is not unstable in the aquatic environment.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you disagree to perform the test as requested. You have provided a new study on ready biodegradation (OECD 301D, June 2018) and state that no further biotic degradation testing is necessary as there is no direct of indirect exposure to the soil compartment.

In response ECHA refers to its observations set out in section 4 above.

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 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. Therefore, the test should be performed at the temperature of 12°C.

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 as described in Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) and R.11 (version 3.0, June 2017).

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).

6. 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 < 1 mg/l (aprox 0.6 mg/l) and high partition coefficient log Kow 7.2, 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 not provided any study record of sediment simulation testing of the registered substance in the registration dossier.

You have sought to adapt this information requirement according to Annex IX, Section 9.2., column 2. You provided the following justification for the adaptation: *"The performance of simulation tests for biodegradation in water and sediment is scientifically unjustified. REACH Regulation (EC) No 1907/2006, Annex IX, Sect. 9.2.1.4., Col. 2, states as follows: "9.2.1.4: The study need not to be conducted: - if the substance is readily biodegradable, or - if direct and indirect exposure of sediment is unlikely. " Direct and indirect exposure of the test item to water and sediment is highly unlikely. Due to the unstable nature of organic peroxides, it can be assumed that upon contact with water and organic matter, the test item undergoes rapid degradation resulting in the formation of respective alcohols and acids. In addition the low adsorption coeffcient (log Koc) of the test item (log Koc=2.69) indicates a low dwell time of the test item in soil and thus a low exposure. Therefore simulation testing for biodegradation in water and sediment was considered not scientifically justified."*

However, ECHA notes that your adaptation does not meet the specific rules for adaptation of Column 2 of Annex IX, Sections 9.2 and 9.2.1.4. for the reasons stated below.

According to Annex IX, Section 9.2.1.4, column 2 of the REACH Regulation, simulation testing on sediment does not need to be conducted if the substance is readily biodegradable or if direct or indirect exposure of sediment is unlikely. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable in OECD 301B test (5% degradation in 28d).

Regarding exposure of sediment, the substance has a low water solubility of <1 mg/l (aprox 0.6mg/l) and high partition coefficient log Kow 7.2 indicating 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 as the exposure estimations that you provided in the Chemical Safety Report (CSR) indicate that there is exposure to sediment in a number of your exposure scenarios (e.g. ES 4, ES 5). ECHA therefore considers that you have not demonstrated that sediment exposure is unlikely. ECHA notes also 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 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.

Moreover, ECHA notes that the hydrolysis is not rapid but moderate or slow following the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6. ECHA notes that you concluded in IUCLID dossier that the half-life at pH = 4, 7 and 9 at 20 °C are 40 hours, 80 hours and 109 hours, respectively. The value used for chemical safety assessment is DT50 = 127 hours at 12 °C, pH 4. Hence, ECHA concludes that the substance is not unstable in the aquatic environment.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you disagree to perform the test as requested. You have provided a new study on ready biodegradation (OECD 301D, June 2018) and state that no further biotic degradation testing is necessary as there is no direct of indirect exposure to the soil compartment. Lastly you note that a new study on a read-across substance (according to OECD 308) is being

conducted.

In response ECHA refers to its observations set out in section 4 above. Additionally, ECHA considers that the mere fact that a registrant of another substance was conducting a test on sediment simulation is not sufficient to address the current data gap in your registration dossier for this information requirement.

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 and anaerobic transformation in aquatic sediment systems (test method EU C.24. / OECD TG 308) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.4.

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. Therefore, the test should be performed at the temperature of 12°C.

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 as described in Guidance on information requirements and chemical safety assessment R.7b (version 4.0, June 2017) and R.11 (version 3.0, June 2017).

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.

Notes for your consideration (for Sections 4, 5 and 6)

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 detailed above is 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. Identification of degradation products (Annex IX, Section 9.2.3.)

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.

In the technical dossier you have identified degradation products from the hydrolysis study (tert-butyl hydroperoxide and cyclohexanone). However, this information does not provide the information required by Annex IX, Section 9.2.3., because it covers only abiotic degradation, however, no information on biotic degradation products is available.

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 in OECD 301B test (5% degradation in 28d) as also discussed in sections 4. – 6. above.

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 further information on the degradation products. ECHA considers that this information is needed in relation to the PBT/vPvB assessment and risk assessment.

In your comments you expressed your overall disagreement with conducting further degradation studies. You additionally referred to the read-across justification provided during your comments on the initial draft decision and to an OECD 308 study on the suggested analogue substance, which has been conducted by the registrant of the analogue substance. You indicated that in this study there were difficulties in identifying the degradation products. ECHA notes that the read-across justification is not available in the dossier. Additionally, ECHA considers that the mere fact that a registrant of another substance was conducting a test on sediment simulation is not sufficient to address the current data gap in your registration dossier for this information requirement.The evaluation of all the new information provided in the update(s) of the registration dossier, submitted after the final decision has been sent to you, will only be performed at the follow-up evaluation stage, pursuant to Article 42 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.

Regarding appropriate and suitable test method, the methods will have to be substance-specific. When analytically possible, identification, stability, behaviour, molar quantity of metabolites relative to the parent compound should be evaluated. In addition, degradation half-life, log Kow and potential toxicity of the metabolite may be investigated. You may obtain this information from the simulaion study(ies) requested in this decision (requests 4 to 6), or by some other measure. You will need to provide a scientifically valid justification for the chosen method.

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.) by using an appropriate and suitable test method, as explained above in this section.

Notes for your consideration

Before providing the above information you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), Chapter R.7b., Sections R.7.9.2.3 and R.7.9.4. These guidance documents explain that the data on degradation products is only required if information on the degradation products following primary degradation is required in order to complete the chemical safety assessment. Section R.7.9.4. further states that when substance is not fully degraded or mineralised, degradation products may be determined by chemical analysis.

8. Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.)

"Bioaccumulation in aquatic species, preferably fish" is a standard information requirement as laid down in Annex IX, Section 9.3.2.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 not provided any study record of bioaccumulation in aquatic species in the dossier that would meet the information requirement of Annex IX, Section 9.3.2.

You have sought to adapt this information requirement according to Annex IX, Section 9.3.2., column 2. You provided the following justification for the adaptation: "*The performance of a test for bioaccumulation in aquatic species, preferably fish, is scientifically unjustified. REACH Regulation (EC) No 1907/2006, Annex IX, Sect. 9.3.2, Col. 2, states as follows: "9.3.2 The study need not be conducted if: - the substance has a low potential for bioaccumulation (for instance a log Kow <= 3) and/or a low potential to cross biological membranes, or - direct and indirect exposure of the aquatic environment is unlikely. " Direct and indirect exposure of the test item to water is highly unlikely. Due to the unstable nature of organic peroxides, it can be assumed that upon contact with water and organic matter, the test item undergoes rapid degradation resulting in the formation of*

respective alcohols and acids. Therefore, the test substance was considered to have no bioaccumulation potential."

However, ECHA notes that your adaptation does not meet the specific rules for adaptation of Annex IX, Section 9.3.2., column 2 because the reported partition coefficient log Kow is 7.2 indicating potential for bioaccumulation, i.e. the log Kow is > 3.

Moreover, ECHA notes that the substance is not readily biodegradable (degradation in OECD 301B test 5% in 28d) and the hydrolysis is not rapid but moderate or slow following the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO (2000)6. ECHA notes that you concluded in IUCLID dossier that the half-life at pH = 4, 7 and 9 at 20 °C are 40 hours, 80 hours and 109 hours, respectively. The value used for chemical safety assessment is DT50 = 127 hours at 12 °C, pH 4. Hence, ECHA concludes that the substance is not unstable in the aquatic environment.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you disagree to perform the test as requested. You have noted that the lead registrant to an analogue substance (CAS 6731-36-8) is probably planning to submit a testing proposal on bioaccumulation and you further claim that due to no exposure to the aquatic compartment no further testing on bioaccumulation on the registered substance is necessary.

In response ECHA considers that the mere fact that a registrant of another substance is probably planning to submit a testing proposal on bio-accumulation is not sufficient to address the current data gap in your registration dossier for this information requirement.

ECHA further notes, that based on the data available in the dossier, the substance is not readily biodegradable, is poorly water soluble (not highly insoluble) and potentially highly adsorptive, indicating that all the compartments (water, sediment and soil) are relevant for this kind of substance. In the exposure scenarios as presented in the CSR there were several RCR's close to [redacted] (for water, sediment and soil compartments) for several exposure scenarios e.g. 4 and 5, indicating that the exposure cannot be considered to be non-existent for any of these compartments.

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.7c* (version 3.0, June 2017) bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to cover the standard information requirement of Annex IX, Section 9.3.2. ECHA Guidance defines further that results obtained from a test with aqueous exposure can be used directly for comparison with the B and vB criteria of Annex XIII of REACH Regulation and can be used for hazard classification and risk assessment. Comparing the results of a dietary study with the REACH Annex XIII B and vB criteria is more complex and has higher uncertainty. Therefore, the aqueous route of exposure is the preferred route and shall be used whenever technically feasible. If you decided to conduct the study using the dietary exposure route, you shall provide scientifically valid justification for your decision. You shall also attempt to estimate the corresponding BCF value from the dietary test data by using the approaches given in

Annex 8 of the OECD 305 TG and in OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation, ENV/JM/MONO (2017)16. In any case you shall report all data derived from the dietary test as listed in the OECD 305 TG.

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:

Bioaccumulation in fish: aqueous or dietary bioaccumulation fish test (test method: OECD TG 305)

Notes for your consideration

Before conducting the above test you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment* (version 3.0, June 2017), Chapter R.11.4. and Figure R.11-4 on the PBT assessment for further information on the integrated testing strategy for the bioaccumulation assessment of the registered substance. In particular, you are advised to first conclude whether the registered substance may fulfil the REACH Annex XIII criteria of being persistent or very persistent, and then to consult the PBT assessment for Weight-of-Evidence determination and integrated testing strategy for bioaccumulation assessment. You should revise the PBT assessment when information on bioaccumulation is available.

9. Identification of PNEC and risk characterisation (Annex I, Section 3.3.1. and 6.): revise PNECs for freshwater, marine water, , freshwater sediment, marine sediment and soil using the assessment factors recommended by ECHA and revise the risk characterisation accordingly *or* provide a detailed justification for not using the recommendations of ECHA guidance in PNEC derivation.

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

Annex I, Section 3.3.1. of the REACH Regulation requires to establish a PNEC for each environmental sphere based on the available information and to use an appropriate assessment factor to the effect values.

The ECHA *Guidance on information requirements and chemical safety assessment,* Chapter R.10 provides further details and specifically provides default assessment factors that should be applied to derive PNECs.

Further, pursuant to Annex I, Section 3.3.2. if it is not possible to derive the PNEC, then this shall be clearly stated and fully justified.

You have used only short-term data and an assessment factor of 100 is used for the calculation of PNEC aquatic.
ECHA notes that according ECHA *Guidance on information requirements and chemical safety assessment,* Chapter R.10 (May 2008), the recommended assessment factor to apply when calculating PNEC for freshwater using only short-term data is 1000 (see also footnote 1 of

Annex I, section 3.3.1. of the REACH Regulation indicating that an assessment factor of 1,000 is typically applied to the lowest of three L(E)C50 values).

You have provided the following justification in the IUCLID dossier: "*OECD GLP freshwater acute (fish, daphnia and algae) and chronic (algae) data are available. The PNEC freshwater was derived the most sensitive short-term aquatic toxicity test for the aquatic compartment, which was the short-term toxicity to algae. The test revealed an ErC50 of > 0.5 mg/L and NOEC of > 0.5 mg/L both expressed as actual concentration. As worst case the ErC50 was considered to be 0.5 mg/L. An assessment factor of 100 was applied (according to organic peroxides consortium's position paper* [redacted] *see also attachment in IUCLID section 13). Equivalently according to EU TGD (2003) PNEC freshwater is set at 1/100 of water solubility. Water solubility is considered to be 0.5 mg/L.*"
However, ECHA notes, that there is no [redacted] attached to the IUCLID dossier in section 13. Moreover, ECHA Guidance *Guidance on information requirements and chemical safety assessment,* Chapter R.10 (May 2008) notes that a long-term test has to be carried out for substances showing no toxicity in short-term tests if the log Kow > 3 and if the PEClogcal/regional is > 1/100th of the water solubility.

In your comments to the draft decision according to Article 50(1) of the REACH Regulation you agree to provide the information as requested.

As explained above, the information provided on PNEC for the registered substance in the chemical safety report does not meet the general requirements for preparing a chemical safety report as described in Annex I, Section 3.3.1.

Consequently, you are given two options: You shall revise the PNECs derived for freshwater, marine water, freshwater sediment, marine sediment and soil by applying the assessment factors recommended by the ECHA *Guidance on information requirements and chemical safety assessment,* Chapter R.10 (May 2008) that are appropriate in these cases. Subsequently, you shall re-assess related risks.

In the alternative, you shall, in accordance with Annex I, Section 3.3.1. and ECHA *Guidance on information requirements and chemical safety assessment,* Chapter R.10., provide a full justification for the PNECs derived for freshwater, marine water, freshwater sediment, marine sediment and soil provided in the chemical safety report by specifying how the following has been taken into account:

a) Intra- and inter-laboratory variation of toxicity data;
b) Intra- and inter-species variations (biological variance);
c) Short-term to long-term toxicity extrapolation;
d) Laboratory data to field impact extrapolation.

A justification for varying the assessment factor could include one or more of the following:
- evidence from structurally similar compounds which may demonstrate that a higher or lower factor may be appropriate.
- knowledge of the mode of action as some substances by virtue of their structure may be known to act in a non-specific manner. A lower factor may therefore be considered. Equally a known specific mode of action may lead to a higher factor.

the availability of data from a variety of species covering the taxonomic groups of species across at least three trophic levels. In such a case the assessment factors may only be lowered if multiple data points are available for the most sensitive taxonomic group (i.e. the group showing acute toxicity more than 10 times lower than for the other groups).

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to revise PNECs for freshwater, marine water, freshwater sediment, marine sediment and soil using the default assessment factors and other recommendations of ECHA Guidance R.10 for PNEC derivation and to revise the risk characterisation accordingly *or* provide a detailed justification for not using the recommendations of ECHA Guidance R.10 for PNEC derivation.

Notes for your consideration

The results of the studies requested with this decision shall be taken into account when revising the PNECs.

Deadline of the decision

In the comments to the draft decision you requested extension of the decision deadline to 36 months because of "*the substance class of peroxyketals is very challenging to assess in regard to biodegradation*." In the draft decision communicated to you the time indicated to provide the requested information was 25 months from the date of adoption of the decision. The decision deadline was therefore modified accordingly.

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 01 March 2018.

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 amended the request(s), but amended the deadline.

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-65 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 requests in this decision 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.