Helsinki, 07 December 2022

Addressees
Registrants of Phenol, 4-methyl-, reaction products with dicyclopentadiene and isobutylene listed in the last Appendix of this decision

Registered substance subject to this decision (the Substance)
Substance name: Phenol, 4-methyl-, reaction products with dicyclopentadiene and isobutylene
EC/List number: 271-867-2
CAS RN: 68610-51-5

Decision number: Please refer to the REACH-IT message which delivered this communication (in format SEV-D-XXXXXXXXXX-XX-XX/F)

DECISION ON SUBSTANCE EVALUATION

Under Article 46 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below:

A. Information required on constituent Type A n=1 of the Substance to clarify the potential risk related to PBT/vPvB

1. **Water solubility (test method OECD TG 105, column elution method) (Request A.1)**.

2. **Simulation testing on ultimate degradation in surface water (Aerobic Mineralisation in Surface Water – Simulation Biodegradation Test; test method OECD TG 309) (Request A.2)**

   The simulation testing must be performed with the following specifications:

   a. At a test temperature of 12ºC;
   b. Using ^{14}C-radiolabelled constituent Type A n=1 of the Substance with the radiolabel located in the most stable part of the molecule. However, if you can demonstrate that radiolabelling is not technically feasible, a non-labelled constituent of the Substance can be used. In this case you must consult the evaluating MSCA before performing the simulation study;
   c. Using a concentration appropriate to also successfully identify and quantify possibly formed transformation and/or degradation products;
   d. The degradation half-life must be determined;
   e. Transformation and/or degradation products relevant for the PBT/vPvB assessment must be identified and quantified at every sampling time;
   f. A mass balance calculation must be included in the test (only if the radiolabelled test material is used);
   g. The total amount of non-extractable residues (NER) must be quantified (if the radiolabelled test material is used) and the reporting of results must include a scientific justification of the used extraction procedures and solvents;
   h. Sterile controls must be included in the test.
   i. The concentration of suspended solids in the surface water sample used must be approximately 15 mg dw/L, or in the range of 10 and 20 mg dw/L.

Only if you can justify that the OECD TG 309 is not technically feasible based on the poor water solubility of the constituent (below 1 µg/L) determined in the Request A.1 and the consequent analytical limitations to quantify the parent compound and/or degradation/transformation products, **one** of the following tests must be performed, depending on your justified choice:

Soil simulation testing (Aerobic and anaerobic transformation in soil; test method OECD TG 307)

OR

Sediment simulation testing (Aerobic and anaerobic transformation in aquatic sediment systems; test method OECD TG 308).

The soil or sediment simulation testing must be performed with the same specifications a. to h. above.

You must consult the evaluating MSCA about the interpretation of results.

If, based on the outcome of Request A.2, the constituent Type A n=1 of the Substance **fulfils the criteria for vP**, according to Annex XIII (Section 1.2.1) of REACH, **OR**, if it can be justified by a read-across from the human health classification of the Substance to the constituent Type A n=1, that the constituent **meets the criteria for T based on human health classification**, according to Annex XIII (Section 1.1.3), **no further testing is required**.

3. **Only if the results from Request A.2 demonstrate that the constituent** Type A n=1 **fulfils the criteria for P but not for vP** according to Annex XIII (Sections 1.1.1 and 1.2.1), **a *Daphnia magna* reproduction test (test method OECD TG 211) (Request A.3)** on the constituent Type A n=1 of the Substance.

4. **Only if the results from the Request A.3 do not allow to conclude whether the constituent** Type A n=1 **fulfils the criteria for toxic (T)** according to Annex XIII (Section 1.1.3), **a Fish Early Life Stage Toxicity Test (test method OECD TG 210) (Request A.4)** on the constituent Type A n=1 of the Substance.

Deadlines

A sequential testing strategy must be applied with multiple deadlines:

Requested information	Conditions when to perform the test	Deadline
A.1 – OECD TG 105	None - always to be performed	**14 March 2025**
A.2 - OECD TG 309 If OECD TG 309 is technically not feasible: OECD TG 307 Or OECD TG 308	None - always to be performed You must consult the evaluating MSCA before performing the simulation study if you use non-labelled test material. By the deadline indicated, you must consult the evaluating MSCA about the interpretation of results.	**08 June 2026**
A.3 – OECD TG 211	**Only if** the results from Request A.2 show that the constituent Type A n=1 of the Substance fulfils the criteria for persistency (P) but not for very persistency (vP) (REACH Annex XIII Sections 1.1.1 and 1.2.1).	**08 March 2027**
A.4 – OECD TG 210	**Only if** the results from Request A.3 do not allow to conclude whether the constituent Type A n=1 of the Substance fulfils the criteria for toxic (T) (REACH Annex XIII Section 1.1.3).	**07 March 2028**

Conditions to comply with the information requested

To comply with this decision, you must submit the information in an updated registration dossier, by each of the deadlines indicated above.

The information must comply with the IUCLID robust study summary format. You must also attach the full study report for the corresponding studies in the corresponding endpoint of IUCLID.

You must update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information.

You will find the justifications for the requests in this decision in the Appendix entitled 'Reasons to request information to clarify the potential risk'.
You will find the procedural steps followed to reach the adopted decision and some technical guidance detailed in further Appendices.

Appeal

This decision may be appealed to the Board of Appeal of ECHA within three months of its notification to you. Please refer to http://echa.europa.eu/regulations/appeals for further information.

Failure to comply

If you do not comply with the information required by this decision by the deadline indicated above, ECHA will notify the enforcement authorities of your Member State.

Authorised[1] under the authority of Mike Rasenberg, Director of 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.

Basis for substance evaluation

The objective of substance evaluation under REACH is to allow for the generation of further information on substances suspected of posing a risk to human health or the environment ('potential risk').

ECHA has concluded that further information on the Substance is necessary to enable the evaluating Member State Competent Authority (MSCA) to clarify a potential risk and whether regulatory risk management is required to ensure the safe use of the Substance.

The ECHA decision requesting further information is based on the following:

(1) There is a potential risk to human health or the environment, based on a combination of hazard and exposure information;
(2) Information is necessary to clarify the potential risk identified; and
(3) There is a realistic possibility that the information requested would allow improved risk management measures to be taken.

The Appendices entitled 'Reasons to request information' describe why the requested information are necessary and appropriate.

Appendix A – Reasons to request information to clarify the potential risk related to PBT/vPvB properties

1. Potential risk

1.1 Potential hazard of the Substance

According to Annex XIII to REACH, the PBT assessment must take account of all relevant constituents of the substance. ECHA Guidance R.11 (ECHA, 2017a) describes relevant constituents as all constituents, impurities and additives present in the substance at levels equal or above 0.1 % (w/w).

The Substance is a UVCB substance consisting of reaction products of p-cresol with dicyclopentadiene (DCPD) and isobutylene. The major constituent 2,2'-(octahydro-4,7-methano-1H-indenediyl)bis[6-tert-butyl-p-cresol] (EC number 255-504-5) and one other constituent, 2,6-di-tert-butyl-p-cresol (EC number 204-881-4) are identified but the main part of the Substance includes unidentified constituents at concentrations < 10% w/w but which are relevant for the PBT assessment.

Based on the available information in the registration dossier on the possible structures, these unidentified constituents can be divided into at least seven different constituent groups (Type A to Type G), defined based on the end groups attached to the cresol-DCPD monomers. Each constituent group includes different isomers due to the multiple possible positions of the phenol rings relative to the DCPD group. Furthermore, all constituent groups except one include also different oligomers with varying number of cresol-DCPD monomers (n=1, n=2, etc.).

Following the assessment of the available relevant information on the Substance, the evaluating MSCA has identified that the potential hazard(s) can be attributed to the constituents referred to as Type A n=1 and Type B n=1 (see Figure 1) of the Substance.

A) B)

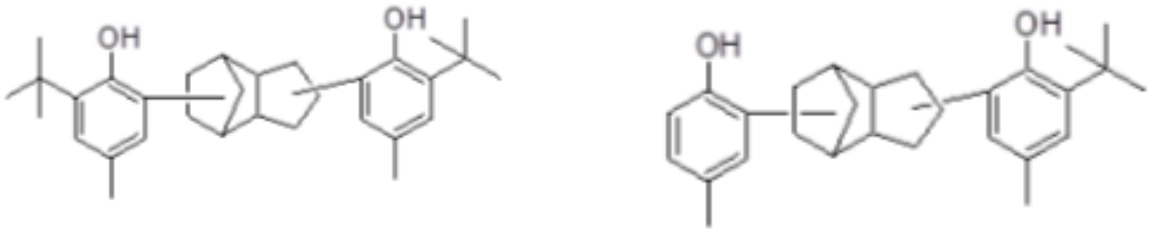

Figure 1: Structural formulas of the constituent A) Type A n=1 and B) Type B n=1

These potential hazards remain to be clarified.

a) Potential P/vP properties

If a substance fulfils the criteria in Section 1.1.1 or 1.2.1 of Annex XIII to REACH, it is considered that it has persistent (P) or very persistent (vP) properties.

For the purpose of the P/vP assessment and to check whether the criteria are fulfilled, the information listed in Section 3.2.1 to Annex XIII, including results from simulation tests, must be considered. If no such data are available, it is necessary to consider the screening information of Section 3.1.1 to Annex XIII, such as QSAR predictions.

The available information suggests that the constituents Type A n=1 and Type B n=1 of the Substance may be persistent or very persistent according to the Annex XIII criteria.

Evidence based on experimental data

The Substance is not readily biodegradable (1% degradation in 28 days in a combined OECD TG 301B and OECD TG 302B test using pre-exposed inoculum) and therefore screens as P and vP according to ECHA Guidance R.11 (ECHA, 2017a).

This information was considered as supporting information since the OECD TG 301 tests are applicable to individual substances, not to mixtures or UVCB/ multiconstituent substances, and it is not possible to conclude on the degradation of individual constituents.

Evidence based on model predictions and other information

According to ECHA Guidance R.11 (ECHA, 2017a), if EPISuite BIOWIN QSAR model 2 or 6 results in a value of < 0.5, and BIOWIN 3 in a value of < 2.25, a substance screens potentially P/vP.

The results of BIOWIN models 2, 3 and 6 for representative constituents of Type A n=1 and Type B n=1 are 0.00-0.42, 1.51-1.91 and 0.0012-0.0039, respectively. Hence, the constituents screen potentially P/vP. The BIOWIN models resulted in slightly lower values for Type A, indicating that the degradation of this constituent could be a bit slower than that of Type B. Type A has a tert-butyl group in both phenyl groups, while Type B has a tert-butyl group only in one of the phenyl group. Therefore, the primary degradation may be more hindered in Type A than in Type B.

Based on the available screening information, the constituents Type A n=1 and Type B n=1 of the Substance may potentially meet the criteria for P or vP.

As the available and current information is not sufficient to draw a conclusion on the hazard, further information on the persistency of the Type A n=1 constituent is needed.

In your comments on the draft decision, you agreed that the potential P property at the constituent level needs to be further investigated.

b) Potential B/vB properties

If a substance fulfils the criteria in Section 1.1.2 or 1.2.2 of Annex XIII to REACH, it is considered that it has bioaccumulative (B) or very bioaccumulative (vB) properties.

For the purpose of the B/vB assessment and to check whether the criteria are fulfilled, the information listed in Section 3.2.2 of Annex XIII must be considered, including bioconcentration factor (BCF) values.

Evidence based on experimental data

- In the registration dossier, you reported a log Kow of 7.93 measured for constituents with n=1 in a slow-stirring method test (OECD TG 123) using the whole UVCB Substance. Based on the information on molecular formula and molecular weight in the robust study report, the n=1 constituent measured in the test refers to the major constituent group, i.e. Type A n=1.

  The only structural difference between constituents Type A n=1 and Type B n=1 is the number of tert-butyl groups: Type A n=1 has two tert-butyl groups (one at each phenol ring) while Type B n=1 has only one tert-butyl group.

  Therefore, the log Kow values of both constituent types are expected to be similar, the constituent Type B n=1 likely having a slightly lower log Kow. This is supported by the

KOWWIN QSAR model which predicts log Kow values of 8.64 and 8.06 for representative constituents of Type A n=1 and Type B n=1, respectively.

Considering the measured log Kow of 7.93 for the Type A n=1, the KOWWIN model seems to slightly overestimate the log Kow value of the constituents.
Hence, both constituents Type A n=1 and Type B n=1 have a log Kow >4.5 and thus, screen potentially B/vB.

- In an OECD TG 305 dietary study with a mixture of constituents Type A n=1 and Type B n=1 of the Substance, growth and lipid corrected BMF_{kgL} values of 0.045 and 0.14 were reported for Type A n=1 and Type B n=1, respectively. The reported growth corrected depuration rates (k_{2g}) were 0.037 and 0.076 day^{-1}, and the growth corrected depuration half-lives ($t_{1/2}$) were 18.7 and 9.14 days for Type A n=1 and Type B n=1, respectively.

  The evaluating MSCA re-ran the kinetic analysis for the data of this study using the bcmfR R-Package (v0.4-18) and obtained slightly different results for Type B n=1, due to selecting a different fit (Ln-transformed data instead of non-transformed data) as the best one for the k_2 calculation. The BMF_{kgL} was 0.148, and the k_{2g} and growth corrected $t_{1/2}$ were 0.053 day^{-1} and 12.99 days, respectively.

  The evaluating MSCA calculated tentative BCF values with the models (Methods 1-3) included in the OECD BCF Estimation Tool (Version 2)[2] and using as input values the experimental k_{2g} and BMF values and other data from the dietary OECD TG 305 study as well as the measured log Kow of 7.93 for both constituent types:

  For Type A n=1 the calculated tentative BCFs are in the range of 476-39869 L/kg with the Method 1 (the median of the values being 9762 L/kg and 10 out of the 13 BCFs above 5000), 14276 L/kg with the Method 2 and 1009 L/kg with the Method 3.

  For Type B n=1 the calculated tentative BCFs are in the range of 333-27908 L/kg with the Method 1 (the median of the values being 6834 L/kg and 10 out of the 13 BCFs above 5000), 9233 L/kg with the Method 2 and 2710 L/kg with the Method 3.

In the draft decision sent for your commenting, ECHA concluded that there seemed to be sufficient information to consider that both constituents Type A n=1 and Type B n=1 are vB, based on a weight of evidence assessment taking into account the low k_{2g} values determined for the constituents in the dietary OECD TG 305 study and the high tentative BCFs mostly above 5000.

In your comments to the draft decision, you disagreed with this conclusion as your assessment of the available information concludes that considering i) the BMF values, (ii) the tentative BCF values calculated with the Method 3 and (iii) the BCFs estimated with BCFBAF QSAR, the Type A is not-B and Type B can be considered B but not vB:

(i) You commented that following the regression analysis by Inoue et al (as defined in the OECD Guidance Document on Aspects of OECD TG 305 on Fish Bioaccumulation - OECD, 2017), a BMFkgl > 1 allows the clear categorization of a test chemical as highly bioaccumulative (BCF would be > 5000 L/kg) and a BMFkgl < 0.1 the clear categorization as not bioaccumulative (BCF would be < 2000 L/kg). Therefore you claim that the constituent Type A with a BMFkgl of 0.0449 can be categorized as not-

[2] Available at: https://www.oecd.org/chemicalsafety/testing/section-3-environmental-fate-behaviour-software-tg-305.htm (Accessed on 22 October 2021)

B with a BCF < 2000 kg/L, while constituent Type B with a BMFkgl of 0.140 has to be regarded as B with a BCF < 5000 L/kg.

ECHA notes that in Annex XIII to REACH no criteria for dietary BMF values in fish are indicated. ECHA agrees with your comment that according to the OECD Guidance Document (OECD, 2017), a dietary BMF>1 determined in an OECD TG 305 study is a clear indication of high bioaccumulation potential. However, the guidance document does not state that a dietary BMF < 0.1 would be a clear indication of a very low bioaccumulation potential, instead a BMF < 0.01 is indicated for this. According to OECD (2017) BMF values < 1 but > 0.01 are not clear-cut, and tentative BCFs are recommended to be calculated. Therefore, ECHA does not agree with your conclusion that based on the BMF values the constituent Type A is not-B and the constituent Type B is not vB.

(ii) You also stated that the results for both constituents are not "clear-cut" as the BMFs are below 1 but not below < 0.01. Therefore, for the purposes of classification and risk assessment, you also calculated tentative BCFs using the above-mentioned OECD BCF Estimation Tool. The tentative BCFs you calculated are very close to the ones calculated by the evaluating MSCA for both constituents types, the small differences being due to some differences in the input values used.

However, in your opinion the constituent Type A is outside the indicative applicability domain of the Methods 1 and 2 of the OECD BCF Estimation Tool as the assimilation efficiency in the OECD TG 305 study was below 0.1.

You further stated that according to the OECD (2017), for substances that have a large molecular weight, a high log Kow and low study assimilation efficiency, the Methods 1 and 2 of the OECD BCF Estimation Tool may be less reliable. According to you, the Method 3 should be preferred for these substances, even when the test species differs from the species used in the training set studies (carp). You point out that as the BMF values were corrected for growth and lipid content, the variability when comparing measured BCFs for different species is reduced. You conclude that for both Type A and Type B, the tentative BCFs estimated by Method 3 should be preferred.

ECHA notes that in OECD (2017), the indicative applicability domains described for the Methods 1 and 2 of the BCF Estimation Tool include substances with log Kow up to 8.2-8.3 and assimilation efficiency approx. > 0.1. Also, it is indicated that the Methods 1 and 2 may be less reliable for substances that are molecularly large or bulky (e.g., more than two aromatic rings and fully halogenated or have molecular weights > 1100 or maximum molecular lengths > 4.3 nm), have high log Kow (approx. 9 or above) and low observed assimilation efficiency, approx.< 0.1).

ECHA points out that:

- the measured log Kow of Type A n=1 is 7.93 and the log Kow of Type B is expected to be lower, and hence, they are both in the applicability domain.

- the assimilation efficiency for Type B (=0.12) observed in the dietary OECD TG 305 study falls inside the applicability domain whereas the assimilation efficiency was lower for Type A (=0.03) and is outside the indicative applicability domain of the methods. Hence, the tentative BCF values for Type A may have more uncertainty.

  However, ECHA notes that in the OECD TG 305 study, the concentration of Type A in the feed was high (932 µg/g) and in the upper limit of the range (1-1000 µg/g)

cited in the test guideline as a workable concentration range. According to OECD (2017), concentrations near the higher end of this range should be avoided if possible, because for some substances, such high concentrations may lead to difficulties in achieving sufficient homogeneity and bioavailability in the feed.

According to OECD TG 305, if using solvent in the spiking of the food, crystallisation of the test substance may occur when the solvent is removed. In the available OECD TG 305 with the constituents Type A and Type B, the constituents were first dissolved in ethanol and then in corn oil. Ethanol was removed by evaporation from this stock solution. It cannot be excluded that crystallisation of the constituents, especially of Type A, present at higher concentration in the final spiked food than Type B (mean concentration in feed 689 µg/g), occurred during the preparation of the test food. This could have led to lower bioavailability of Type A, and hence, the assimilation efficiency measured in the test may underestimate the real uptake of the constituent.

- the molecular weights of the constituents Type A n=1 and Type B n=1 are 460 and 405 g/mol, respectively. They are both well below the limit of 1100 g/mol indicated in OECD (2017) for very large molecules.

  Furthermore, ECHA Guidance R.11 (ECHA, 2017a) mentions that a log Kow > 10, a molecular weight > 700 g/mol and an average maximum diameter of the molecule (Dmax aver.) > 1.7 nm may be used as possible indicators of limited uptake leading to not-vB properties.

  The evaluating MSCA calculated the maximum distances for example isomers of Type A and Type B with the MolView programme. For Type A it was calculated for two isomers, for the one reported as the main constituent and for another one that would be the longest one due to the position of the phenol groups in the dicyclopentadiene. (a) For the longest isomer of Type A, the maximum distance is 1.8 nm, and hence, it is just above the limit indicated for DMax aver. in ECHA (2017a) for limited uptake; (b) For the other isomer and for Type B, the distance is below 1.7 nm. These values are also well below the limit of 4.3 nm for maximum molecular length indicated in OECD (2017) for very large molecules.

  Note: According to ECHA (2017a), the threshold value of 1.7 nm for the Dmax aver. was derived using the descriptor Dmax from OASIS and based on Environment Agency (2009) it appears that the use of different software tools could lead to variable results for the same substance. In conclusion, the maximum distance values calculated by the evaluating MSCA for the constituents are not directly comparable with the indicator value Dmax aver. mentioned in the ECHA (2017a).

In conclusion, considering the predicted molecular length, the molecular weight of 405-460 g/mol, and the measured log Kow value of 7.93 being well below 10, the uptake of the constituents Type A n=1 and Type B n=1 are not expected to be very limited. Therefore, ECHA considers that the Methods 1 and 2 of the BCF Estimation Tool can be considered in the weight of evidence assessment of these constituents.

Regarding Method 3, its applicability to other fish species than carp is not known (OECD, 2017). As the rainbow trout was used as test species in the available OECD TG 305, the applicability of Method 3 for tentative BCF values is uncertain. For example, Wassenaar et al. (2020) assessed the impact of different test characteristics on BCF values and their variation using an extensive dataset of bioconcentration

studies and found that test species type at sub-cohort level had a significant effect in the BCF values. For the group of Ostariophysi, which is mainly represented by the common carp, lower BCF values were observed, than for Neoteleostei and Protacanthopterygii groups, which are mainly represented by the guppy, high-eyes medaka and the rainbow trout. The authors suggest that the differences between species could be related e.g. to differences in the ventilation rate, which affects uptake, and metabolism, which in turn affects depuration.

Therefore, ECHA disagrees with your comment that the Method 3 should be preferred over Methods 1 and 2 in the case of the two constituents.

(iii) You also reported that the BCFBAF v3.01 QSAR model predicts a BCF of 733 L/kg for Type A (n=1) and a BCF of 2420 L/kg for Type B (n=1) following a regression-based estimation. In addition, you report estimated BAF (Arnot-Gobas method, upper trophic level) of 1220 L/kg for Type A (n=1) and 1330 L/kg for Type B (n=1) and estimated growth corrected half-lives of 8.26 and 3.67 days, respectively.

ECHA highlights that:
* When using the measured log Kow of 7.93 as input in the QSAR model, a BCF of 2794 L/kg is predicted for both Type A and Type B with the regression-based method.

* For Type A, the Arnot-Gobas method results in BCF values in the range of 177-270 L/kg (upper, mid and lower trophic levels) when including biotransformation estimates and in BCF of 3790 L/kg (upper trophic level) when assuming zero biotransformation. For Type B, the BCFs predicted by the Arnot-Gobas method are also very similar (BCFs 74-112 with biotransformation estimations and 3790 with zero biotransformation).

The Arnot-Gobas method seems to overestimate the biotransformation rate as the depuration half-lives observed in the dietary study are much higher (19 and 13 days) than the biotransformation half-lives predicted by the model (8 and 3 days). Therefore, the BCFs predicted including the biotransformation rate estimations are not considered reliable. In conclusion, the BCF values predicted by BSFBAF QSAR model support that both Type A and Type B are bioaccumulative.

ECHA also notes that another substance, Dechlorane plus (EC236-948-9), covering its anti- and syn-isomers, has been concluded as vB based on the long depuration half-life indicative of a BCF > 5000 L/kg, by comparison with substances that have been concluded to be vB under REACH (ECHA, 2017c). The growth-corrected depuration half-life determined for Dechlorane Plus in a non-standard dietary study with rainbow trout was around 36 days for the anti- isomer and 58 days for the syn- isomer. The BMF_{kgL} values were 0.022 and 0.12 for anti- and syn-isomers, respectively. Hence, the BMF values are very similar to those determined for Type A and Type B constituents, while the depuration half-lives were higher for Dechlorane Plus than for the two constituents of the Substance (19 and 13 days for Type A and Type B, respectively). However, some of the other substances concluded to be vB and compared with Dechlorane Plus in the SVHC identification Support Document (ECHA, 2017c) have depuration half-lives of 3-4 days (musk xylene) or approx. 20 days (D5).

Therefore, ECHA considers that based on a weight of evidence assessment taking into account the low k_{2g} values determined for the constituents in the dietary OECD TG 305 study and the high tentative BCFs mostly above 5000, there is sufficient information to consider that the constituents Type A n=1 and Type B n=1 are vB.

c) Potential T properties

If a substance fulfils the criteria in Section 1.1.3 of Annex XIII to REACH, it is considered that it fulfils the toxicity (T) criterion.

For the purpose of the T assessment and to check whether the criteria are fulfilled, the information listed in Section 3.2.3 of Annex XIII must be considered, such as the results of long-term toxicity tests.

Evidence based on experimental data

- You have self-classified the Substance as Toxic for reproduction, category 2. The classification is based on the results of a prenatal developmental toxicity study (OECD TG 414) in New Zealand White rabbits performed with the Substance. However, it cannot be concluded whether the constituent Type A n=1 warrants the same classification based on the available information.

- You reported two long-term toxicity studies (Unnamed, 2015 and Unnamed, 2017) with *Daphnia magna* following OECD TG 211 for the Substance. In both studies, the definitive test included only one test concentration prepared using the WAF approach.
  - In Unnamed (2015) a statistically significant reduction in the number of offspring per surviving parent was observed, and a 21-day NOELR of < 1 mg/L loading rate for reproduction is reported. The measured concentrations were either below or around the concentration of the lowest calibration solution (0.5 µg/L).
  - In Unnamed (2017) a 9.7% reduction in the mean number of living offspring per surviving parent was observed at a loading rate of 100 mg/L but the difference compared to the control group was not statistically significant. The measured test concentrations were below the limit of detection (0.75 µg/mL).

- The registration dossier also includes a long-term toxicity test with fish (OECD TG 210) at a loading rate of 1 mg/L and a toxicity test with algae (OECD TG 201) at a nominal concentration of 0.2 mg/L (solvent used) for the Substance. No effects were observed in these tests. In the OECD TG 210 fish test, the measured concentrations were below or around the concentration of the lowest calibration solution, i.e. below 0.5 µg/L. In the OECD TG 201 algal test, the actual concentrations of the test solutions could not be determined.

Since the available aquatic toxicity tests were performed with the whole UVCB Substance, it is not possible to conclude on the toxicity of individual constituents. The exposure concentrations of individual constituents in the toxicity tests with the UVCB Substance are not known, and therefore, some of the constituents may show effects not observed in the tests with the UVCB Substance when tested alone at higher exposure concentrations.

Evidence based on model predictions and other information

- For constituents Type A n=1 and Type B n=1, the ECOSAR v1.11 QSAR model predicts for fish and daphnia chronic toxicity values below 0.01 mg/L. The predictions are based on the ECOSAR Class "Phenols, Poly" and baseline toxicity for the class Neutral Organics. The Type A n=1 has slightly lower predicted values (0.0000835 and 0.000233 mg/L) than the Type B (0.000228 and 0.000554 mg/L) when using the log Kow values predicted by KOWWIN as input. When using the measured log Kow of 7.93 as input ECOSAR predicts for Type A chronic values in fish and daphnia of 0.00033 and 0.00079 mg/L, respectively.

A chronic value given by ECOSAR QSAR-model is the geometric mean of predicted lowest observed effect concentration (LOEC) and no-observed effect concentration (NOEC). Hence, the predicted NOEC is even lower than the chronic value given by the model.

According to ECOSAR, if the log Kow of the chemical is greater than the endpoint specific cut-offs indicated for the model, then no toxic effects for those endpoints are expected in aquatic organisms when exposed to saturated aqueous solutions of the chemical.

It is noted that the predicted log Kow values of the constituents Type A n=1 (8.6) and Type B n=1 (8.06) are just at the limit or above the cut-off value of 8.0 indicated for the Chronic values of the Phenols, Poly and Baseline toxicity models. However, the measured log Kow of Type A n=1 (7.93) is below the cut-off limit and the actual log Kow of the constituent Type B n=1 is expected to be even lower (as explained above). Therefore, based on the ECOSAR QSAR predictions, the constituents Type A n=1 and Type B n=1 may potentially have chronic aquatic toxicity values below 0.01 mg/L, and hence, are potentially T according to Annex XIII of REACH.

The available and current information is not sufficient to draw a conclusion on the T properties of the constituent Type A n=1 of the Substance. Therefore, further information on the long-term aquatic toxicity of the constituent is needed if it is first confirmed to be P and B/vB but not vPvB.

In your comments on the draft decision, you agreed that the potential T property at the constituent level needs to be further investigated.

1.2 Potential exposure

According to the information you submitted in all registration dossiers, the aggregated tonnage of the Substance manufactured or imported in the EU is in the range of 10 000 to 100 000 tonnes per year.

Furthermore, you reported that release of the Substance during service life and waste stage of the articles may occur from:

a) industrial use: formulation in materials, industrial abrasion processing ([redacted]), formulation of mixtures and in the production of articles for thermoplastic manufacture and as processing aid and industrial abrasion processing with low release rate ([redacted]),
b) outdoor widespread use by professional workers in long-life materials ([redacted]) and
c) indoor widespread use by consumers in long-life materials ([redacted]).

Therefore exposure to environment cannot be excluded.

1.3 Identification of the potential risk to be clarified

Based on all information available in the registration dossier and the QSAR modelling performed by the evaluating MSCA, the constituents Type A n=1 and Type B n=1 of the Substance may be PBT/vPvB substances.

The information you provided on manufacture and uses demonstrates a potential for exposure of the environment.

Based on this hazard and exposure information the Substance poses a potential risk to the environment.

As explained in Section 1.1 above, the available information is not sufficient to conclude on the hazard and in particular P/vP and T properties.

Consequently, further data is needed to clarify the potential risk related to PBT/vPvB properties of the constituents Type A n=1 and Type B n=1 of the Substance.

1.4 Further risk management measures

If the properties(s) of the Substance are confirmed, the evaluating MSCA will analyse the options to manage the risk(s).

New regulatory risk management measures could be identification as a substance of very high concern and authorisation/restrictions of the use of the substance for PBT properties.

This would result in stricter risk management measures, such as improved measures at manufacturing sites, better waste management and revised instructions on safe use, if appropriate.

2. How to clarify the potential risk

2.1 Development of the testing strategy

a) Justification

As originally indicated in section 1.1, ECHA considers that the constituents Type A n=1 and Type B n=1 seem to fulfil the criteria for vB according to REACH Annex XIII.

In your comments on the draft decision, you disagreed with ECHA's conclusion (see section 1.1.b) and stated that Type A is not-B and only the constituent Type B should be tested for persistence and toxicity. However, you also commented that if ECHA considers that both constituents seem to be B/vB and that information on persistence is needed for both of them, the Type B should be tested first. As explained in section 1.1 and after considering your comments, ECHA maintains its conclusion that both constituents Type A and Type B can be considered to fulfil the criteria for vB. Therefore, there is a concern on potential PBT/vPvB properties.

Nevertheless ECHA agrees with your proposal to not test the two constituent types together in a simulation study, because this could lead to difficulties in the detection of the constituents in water, soil or sediment, as well as in the determination of transformation/ degradation products and NER.

However, ECHA does not agree with you that the Type B should be tested first. As indicated in section 1.1, based on its structure and the BIOWIN QSAR predictions, the constituent Type A may be more resistant to degradation than Type B. Therefore, ECHA considers that Type A should be tested first in a simulation study as it represents the worst-case for persistency.

Consequently, a testing strategy to clarify whether the constituent Type A n=1 fulfils the criteria for PBT/vPvB according to REACH Annex XIII is described below, while the requests

for Type B included in the original draft decision have been removed. If further information to clarify the PBT/vPvB concern on Type B n=1 is needed, this can be requested in a future Substance Evaluation decision.

In your comments on the draft decision, you agreed that the potential P and T properties, at the constituent level need to be further investigated. However, you suggested to request only the simulation study together with the preliminary water solubility study in the present decision, and address the environmental toxicity testing in a later decision. ECHA disagrees with this proposal as adding conditional requests speeds up the PBT/vPvB evaluation of the Substance.

Therefore, ECHA has maintained the tiered testing strategy in the present decision (i.e., including also aquatic toxicity tests as conditional requests). You must follow the tiered-testing strategy to clarify whether the constituent Type A n=1 fulfils the criteria for PBT/vPvB according to REACH Annex XIII.

b) Description

The requested water solubility (Request A.1) and simulation degradation studies with the constituent Type A n=1 (Request A.2) form the **first tier** in the testing strategy.

A request for a water solubility study has been included in the decision following your comment on the draft decision. The outcome of that study must be used for deciding on the test compartment to be assessed in the simulation study.

If as an outcome of the simulation testing (Request A.2),
- the constituent Type A n=1 fulfills the criteria for vP and the vPvB properties of the Substance are confirmed, no further testing is required.

- the constituent Type A n=1 fulfills the criteria for P only, but not for vP, according to Annex XIII Sections 1.1.1 and 1.2.1 of REACH, further T testing is triggered as a **second tier**, i.e., information on long-term aquatic toxicity is requested.

Within this second tier, the long-term daphnia test (Request A.3) is to be conducted first to clarify whether the criterion for T according to Annex XIII Section 1.1.3 of REACH is met.
If as an outcome of the Request A.3,
- the constituent meets the criterion for T of Annex XIII of REACH, the PBT properties of the Substance are confirmed, and no further testing is required.

- the constituent Type A n=1 does not fulfil the criterion for T, a long-term test in fish is triggered (Request A.4).

Information requests A.1 to A.4 are standard information requirements of REACH and could be subject to a compliance check under Article 41 of REACH. However, since these information requests are based on a potential risk identified for the constituent Type A n=1 of the Substance, and testing is requested to be performed with this constituent type, substance evaluation is an appropriate process.

If further information to clarify the remaining concern is needed, this can be requested in a future Substance Evaluation decision.

In your comments on the draft decision, you highlighted that you have self-classified the

Substance as Repr. 2, and hence, the whole UVCB Substance fulfils the criteria for T according to Annex XIII of REACH. However, as the Substance is a complex reaction mass that contains several different constituents at varying concentrations, the exact composition of the test material is not known, and the physico-chemical properties and toxicity of the constituents are expected to differ from the whole UVCB Substance. Consequently, based on the available information it is difficult to assess which of the constituents caused the effects observed in the tests performed with the whole UVCB Substance. In your comments you also agreed that further information on the toxicity at constituent level is needed.

ECHA notes that if it can be justified by a read-across from the human health classification of the Substance to the constituent Type A n=1, that the constituent meets the criteria for T, based on human health classification, then no further testing to clarify T is required.

2.2 Water solubility (OECD TG 105, column elution method)

a) Aim of the study

There is no measured data on the water solubility of the constituent Type A n=1 of the Substance. In an OECD TG 105 study using the column elution method, the solubility of the whole UVCB Substance was determined to be below 0.01 mg/L (at 20°C) as no levels of the Substance were detected above the limit of quantification (LOQ=0.01 mg/L). For the constituent Type A n=1, when using the measured log Kow of 7.93 as input, the WSKOW (v1.42) and WATERNT (v1.01) QSAR models predict water solubility values of 0.0008 and 0.000006 mg/L, respectively.

The water solubility must be confirmed experimentally to be able to select an appropriate test compartment for the requested degradation simulation study. It is also important to have an accurate value of the water solubility to ensure that concentrations below the water solubility are used in the aquatic toxicity studies requested conditionally in this decision.

b) Specification of the requested study

Test method and test material

You must measure the water solubility according to the OECD TG 105, using the column elution method as it is the most appropriate method for substances with low water solubilities (< 10^{-2} g/L).
The constituent Type A n=1 must be used as test material.

In your comments on the draft decision, you proposed that the water solubility test could be performed with Type B n=1 and the result could be read across to Type A, because of the similarity of the constituents, their water solubilities should not be very different and should be at a very low level.

However, as explained in the section 2.1, ECHA considers that the simulation study, and consequently also the conditional aquatic toxicity studies, should be performed first for Type A n=1, as it represents the worst case for persistency. Therefore, it is reasonable and most cost- and time efficient to perform the water solubility study also with the same constituent, because the Type A could have slightly lower water solubility than Type B, and only one constituent type needs to be synthetised for the tests requested in this decision.

c) Alternative approaches and how the request is appropriate to meet its objective

The water solubility study with the constituent Type A n=1 of the Substance is:

1. Appropriate, because there is no measured data on the water solubility of the constituent Type A n=1 of the Substance.
2. Suitable and necessary to obtain information which will allow selecting an appropriate test compartment for the requested degradation simulation test (Request A.2) and to ensure that concentrations below water solubility are used in the conditionally requested aquatic toxicity tests (Requests A.3 and A.4);
3. The least onerous measure, because there is no equally suitable alternative methodology available to obtain the information that would clarify the potential hazard.

2.3 Aerobic Mineralisation in Surface Water – Simulation Biodegradation Test (OECD TG 309)

OR if OECD TG 309 is not technically feasible, **Aerobic and anaerobic transformation in soil (OECD TG 307), OR, Aerobic and anaerobic transformation in aquatic sediment systems (OECD TG 308)**

a) Aim of the study

As detailed in Section 1.1 above, further information on degradation of the constituent Type A n=1 is required to conclude on its persistency. The requested surface water simulation test, or if based on the outcome of the Request A.1 it is not technically feasible, the soil or water-sediment simulation test, will allow to obtain degradation half-lives of the constituent Type A n=1 of the Substance and to identify transformation and/or degradation products.

b) Specification of the requested study

Selection of the test compartment

According to Section R.11.4.1.1.1, page 44 of ECHA Guidance R.11 (ECHA, 2017a), in the persistence assessment, a conclusion must be derived for all environmental compartments. The specific concern for persistency is normally present for the environmental compartment for which the P/vP criteria are most likely to be met. Exclusion of certain environmental compartments from the P/vP assessment based on absence of exposure may be acceptable only in very exceptional cases and upon justification.

The ECHA Guidance R.11 (ECHA, 2017a) further indicates that testing in the aquatic compartment (OECD TG 309) is normally the preferred first step when there is a need for further information on persistence in the environment as this minimises the potential NER formation, which can confound interpretation of the results from sediment and soil simulation studies (OECD TG 308 and 307). However, when water solubility of a substance is very low (typically <1 µg/L), testing on sediment and/or soil will be preferred, if aquatic simulation degradation testing is not technically feasible due to analytical limitations and low solubility of the test substance.

In your comments on the draft decision, you speculated that ECHA may have requested an OECD TG 309 as a first option because, based on the risk assessment of the Substance, water is currently the most relevant route of exposure. You further mentioned that "*any deviation from this would risk that the results of the simulation study cannot be reliable used to this exposure pathway*". You also assumed that ECHA calls for coordination with the evaluating MSCA on this issue.

ECHA highlights that the simulation study is requested solely to clarify a potential risk of PBT/vPvB properties of the constituent Type A n=1, not to refine the environmental exposure assessment of the Substance. The conditions under which an OECD TG 309 study can be considered not technically feasible are indicated in the decision, and hence, ECHA does not require any mandatory consultation with the evaluating MSCA on the selection of the test system. However, ECHA notes that communication with the evaluating MSCA is possible in case you wish to have a concerted discussion on this issue.

As indicated in the Request A.1, the water solubility of the constituent Type A n=1 is expected to be low. Therefore, you should assess the technical feasibility of performing OECD TG 309. According to ECHA Guidance R.11 (ECHA, 2017a), 'not technically feasible' means that it has been impossible, with allocation of reasonable efforts, to develop suitable analytical methods and other test procedures to accomplish testing in surface water so that reliable results can be generated. Appropriate analytical methods should have a suitable sensitivity and be able to detect relevant changes in concentration (including that of degradation/transformation products).

Hence, if based on the outcome of the Request A.1 you can justify that, due to the poor solubility (below 1 µg/L) of the constituent Type A and consequent analytical limitations to quantify the parent compound and/or degradation/transformation products, simulation testing in surface water is not technically feasible, testing either in water-sediment or soil is considered more appropriate for the constituent.

Furthermore, based on the predicted log Koc values of 8.6 and 6.0 (based on KOCWIN MCI and log Kow methods, respectively), the constituent Type A n=1 has a high tendency to adsorb to organic material.

The EPISuite Level III Fugacity model predicts that the constituent will mainly distribute to sediment (57%) and soil (42%), and only <1% will end up in water if equal emissions to water, soil and air are assumed.

According to the EPISuite STP Fugacity model, when the constituent is released to a sewage treatment plant, 93% will end up in sewage sludge and 6% will remain in the effluent water.

Therefore, sediment and soil are expected to be the most relevant environmental compartments. Since ECHA is currently not aware of any information indicating that the persistence of the constituent Type A n=1 could be higher in one of these compartments, in case OECD TG 309 is technically not feasible, you can choose whether you will perform a soil or water-sediment simulation test. You must justify your choice.

If the simulation study results in the constituent being "not persistent" according to Annex XIII to REACH in the tested compartment and these results are sufficient to conclude on persistency in other environmental compartments, no additional simulation test will be needed. However, if a concern on the persistency in some of the compartments remains, the evaluating MSCA may consider whether further simulation testing needs to be requested in another Substance Evaluation decision.

Test temperature

The test must be performed at 12ºC to represent the average environmental temperature for the EU.

Test material preparation and concentration

The test must be performed using as test material the constituent Type A n=1 of the Substance with ^{14}C-radiolabelling. The radiolabelling must be in the most stable part of the molecule. The same constituent was synthetised for the previously performed OECD TG 305 bioaccumulation test.

In your comments on the draft decision, you considered that, based on your previous communication with laboratories experienced with radiolabelling, it is likely that the constituent Type A cannot be produced as radiolabelled material. ECHA notes that radiolabelling is recommended in the OECD TG 309 as well as in OECD TG 307 and 308, as it allows the measurement of non-extractable residues (NER) and ^{14}CO2, and consequently the determination of full mass balance. Based on the high predicted log Koc values of the constituent Type A (6.0-8.6), formation of NER could be significant, especially in the soil and sediment simulation studies. Lack of such data on its amount could potentially lead to difficulties in interpreting the results of the study. Therefore, ECHA requests to use a radiolabelled test material (at the most stable part of the molecule).

However, if you can demonstrate that radiolabelling is not technically feasible, ECHA agrees that the test can also be conducted with a non-labelled test material using a suitable analytical method. In this case you must consult the evaluating MSCA before performing the simulation study. ECHA emphasises that it is your responsibility:

- to prove the adequacy of the analytical methods according to the requirements of the OECD TG 309, 307 or 308 and
- to ensure that the test performed (i) meets the quality criteria (regarding recovery, repeatability, and sensitivity of the analytical method) of the guideline and (ii) provides results suitable for comparison with the Annex XIII criteria for P/vP of REACH.

You must use a test concentration appropriate to also successfully identify and quantify possibly formed transformation and/or degradation products.

Determination of degradation half-lives

Degradation half-life must be determined for the constituent Type A n=1.

Identification of transformation and/or degradation products

Transformation and/or degradation products relevant for the PBT assessment must be identified and quantified at every sampling time.

Mass balance and quantification of NER

A mass balance calculation must be included in the test (only if the radiolabelled test material is used).

The total amount of non-extractable residues (NER) must be quantified (if the radiolabelled test material is used) and the reporting of results must include a scientific justification of the used extraction procedures and solvents. By default, total NER is regarded as non-degraded substance. However, if reasonably justified and analytically demonstrated a certain part of NER may be differentiated and quantified as irreversibly bound or as degraded to biogenic NER.

Such fractions could be regarded as removed when calculating the degradation half-life(s) (ECHA, 2017a). The Background note on 'Options to address NER in regulatory P

assessment', published on the ECHA website, provides some suggestions for the further refinement[3].

Sterile controls

Sterile controls must be included in the test in order to determine to what extent the test material decrease is due to biotransformation or to potential abiotic losses (e.g. adsorption to test vessel or tubing, formation of non-extractable residues (NER)).

In this context, ECHA notes that it is important to ensure that test conditions in the sterile controls and the active test bottles are as equal as possible. A precondition for conclusion on degradation is that other removal processes are not assessed as degradation. With this aim it is necessary to compare processes observed in sterile controls with those observed in the active test bottles under comparable test conditions.

Therefore, other specifications of the sterile control bottles, such as sampling times, analytical measurements as well as any potential cause of disturbance (such as aeration events) that might affect the distribution of the test substance or that could cause leakage, must be the same as in the active test bottles, to ensure comparability.

The OECD TG 309 gives guidance on the preparation of sterile water controls as well as sterile controls containing water with sediment added in large amounts. The OECD TG 308 does not include instructions for a sterile control, while the OECD TG 307 includes instructions for a sterile control but does not include specific advice on soil sterilisation methods. The OECD TG 307 refers to two references for soil sterilisation methods (OECD, 1993; Stenberg et al., 1996). However, the evaluating MSCA checked these references and found no information on sterilisation of soil samples.

The selection of the sterilisation method may have an effect on the sediment or soil properties. In the case of a sediment study, also the time to perform the sterilisation in the sterile water-sediment controls, e.g. before or after the acclimation period specified in paragraph 31 of OECD TG 308 can affect the sediment properties. Considering the importance of the integrity of the sediment or soil phase to produce meaningful results for comparison to unsterilised conditions, ECHA recommends to use sterilisation methods that have the least impact on the mineral phases and the geochemistry of the sediment or soil.

Therefore, if you perform an OECD TG 308 or TG 307 study, you are advised to consider relevant publicly available information on sterilisation of sediment or soil for technical guidance on the sterilisation methods.

ECHA notes that the OECD TG 308 test (Unnamed, 2010; ECHA, 2018) for decamethylcyclopentasiloxane (EC number 208-764-9), as well as other published water-sediment degradation simulation studies (e.g. Liu et al, 2013; Shrestha et al 2016, 2020) included sterile controls and can provide guidance on the preparation of sterile controls. In these studies the sterilisation was done either by the addition of sodium azide, autoclaving or both. In addition, in another publication (Otte et al, 2018) different methods for sterilisation of marine sediment were compared. Based on Otte et al (2018), thermal sterilisation, gamma radiation and chemical sterilisation have all advantages and disadvantages.

[3] https://echa.europa.eu/documents/10162/13632/bg_note_addressing_non-extractable_residues.pdf/e88d4fc6-a125-efb4-8278-d58b31a5d342

According to Otte et al (2018) autoclaving and gamma radiation lead to a large increase in dissolved organic carbon and have impacts on the mineral phase, while chemical sterilisation seems to be the method that would likely have the least impact on the geochemistry of the sediment phase. However, it should be noted that chemical sterilisation may also affect some sediment properties, e.g., triggering changes in pH. OECD TG 309 also indicates that the sorption characteristics of the sediment may be altered by autoclaving.

Berns et al. (2008) studied the effect of two common soil sterilisation methods (gamma radiation and autoclaving) on two different types of agricultural soils. They concluded that the choice of the sterilisation method strongly depends on the type of study or research questions being asked. For degradation experiments, gamma-sterilised soils are better suited as control soils than autoclaved soils, because they are physically and chemically less altered by the process of sterilisation.

Lees et al. (2018) assessed autoclaving, gamma irradiation, and sodium azide as soil sterilisation methods for use in adsorption/desorption studies. They reported that autoclaving destroyed the soil structure, therefore potentially affecting its sorption behaviour while sodium azide changed the pH of the loam soil solution by 0.53 pH units. Gamma irradiation exhibited least disruption to the tested soils physico-chemical properties. The authors concluded that gamma irradiation was the best available method for sterilising soils in preparation for sorption-desorption experiments, but advocated for a case-by-case basis approach for choosing the best sterilisation in different soil types.

In conclusion, you must explain and justify in the study report the method and procedure used for establishing the sterile controls, and determine the efficiency of the sterilisation by measurements of microbial biomass. The OECD TG 308 indicates that the microbial biomass of both water and sediment must be measured at post-handling, test start and test end, and mentions methods for that. OECD TG 307 indicates that the microbial biomass of soil must be measured initially, during and at the end of the aerobic studies. Finally, ECHA notes that communication with the evaluating MSCA is possible in case you wish to have a concerted discussion on the preparation of the sterile controls.

Amount of suspended solids (only relevant for OECD TG 309)

The amount of suspended solids in the OECD TG 309 pelagic test should be representative of the level of suspended matter (SPM) in EU surface water (approximately 15 mg dw/L). The concentration of suspended matter in the surface water sample used must therefore be approximately 15 mg dw/L and fall in the range of 10-20 mg SPM dw/L, which is considered acceptable according to Section 7.9.4.1 of ECHA Guidance R.7b (ECHA, 2017b).

Request for the full study report

You must submit the full study report which includes:
- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

This will enable the evaluating MSCA to fully and independently assess all the information provided, including the statistical analysis, and to efficiently clarify the potential hazard for the PBT/vPvB properties for the Substance.

c) Alternative approaches and how the request is appropriate to meet its objective

The Request A.2 for a surface water, soil, or water-sediment simulation study with the constituent Type A n=1 of the Substance is:

1. Appropriate, because the test is suitable and necessary to obtain information which will allow clarifying whether the constituent Type A n=1 of the Substance has a half-life in surface water, soil or sediment which fulfils the P or vP criteria of Annex XIII and whether transformation and/or degradation products having potential PBT/vPvB properties are formed under environmental relevant conditions;
2. The least onerous measure, because there is no equally suitable alternative methodology available to obtain the information that would clarify the potential hazard.

2.4 *Daphnia magna* Reproduction test (test method OECD TG 211)

a) Aim of the study

The requested *Daphnia magna* Reproduction test allows to evaluate long-term aquatic toxicity of the constituent Type A n=1 and to confirm whether the constituent fulfils the criteria for toxicity (T) in Annex XIII to REACH.

If based on the results of the requested *Daphnia magna* reproduction study, the constituent fulfils the criteria for T according to Annex XIII, no further testing is required.

If the results do not allow to draw a firm conclusion on whether the constituent meets the criteria for T in Annex XIII of REACH, a long-term toxicity study on fish is required (see Request A.4)

b) Specification of the requested study

Test material and concentration

The test must be performed using the constituent Type A n=1 of the Substance as test material.

Due to the poor water solubility and high tendency to adsorb to organic material the constituent is considered a difficult substance for aquatic toxicity testing, and therefore ECHA recommends you to consult the OECD Guidance Document 23 on Aqueous-Phase Aquatic Toxicity Testing of Difficult Test Chemicals (Second Edition) (OECD, 2019), to help to achieve and maintain the required exposure concentration.

Request for the full study report

You must submit the full study report which includes:

- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

This will enable the evaluating MSCA to fully and independently assess all the information provided, including the statistical analysis, and to efficiently clarify the potential hazard for the PBT/vPvB properties for the Substance.

c) Alternative approaches and how the request is appropriate to meet its objective

In your comments on the draft decision, you highlighted that you are currently revising the CSR of the Substance and that "*the relevant exposure pathway may change*", in which case a terrestrial toxicity study might be useful. ECHA reminds that the aquatic toxicity testing in this decision is requested to obtain information which will allow clarifying whether the constituent Type A n=1 of the Substance fulfils the Annex XIII criteria for T. Annex XIII of REACH has criteria only for aquatic toxicity and human health classification. Therefore, if further information on the environmental toxicity of the constituent is needed, aquatic toxicity testing is considered the most efficient first step to clarify whether the criterion for T in Annex XIII is fulfilled.

If it is not possible to conclude whether the constituent fulfils the criteria for T based on human health classification (see Section 2.1.b above), Request A.3 for *D. magna* Reproduction test with the constituent Type A n=1 of the Substance is:

- Appropriate, because the test is suitable and necessary to obtain information which will allow clarifying whether the constituent of the Substance fulfils the Annex XIII criteria for T;
- The least onerous measure, because there is no equally suitable alternative methodology available to be used as a first step of aquatic toxicity testing before going to vertebrate testing (fish) to obtain the information that would clarify the potential hazard.

2.5 Fish Early Life Stage Toxicity Test (OECD TG 210)

a) Aim of the study

The requested Fish Early Life Stage Toxicity Test allows to evaluate the long-term aquatic toxicity of the constituent Type A n=1 and to confirm whether the constituent fulfils the criteria for toxicity (T) in Annex XIII to REACH in case it is not possible to draw a firm conclusion on the toxicity based on the outcome of the OECD TG 211.

b) Specification of the requested study

Test material and concentration

The test must be performed using the constituent Type A n=1 of the Substance.

Due to the poor water solubility and high tendency to adsorb to organic material the constituent is considered a difficult substance for aquatic toxicity testing, and therefore ECHA recommends that you consult the OECD Guidance Document 23 on Aqueous-Phase Aquatic Toxicity Testing of Difficult Test Chemicals (Second Edition) (OECD, 2019), to help to achieve and maintain the required exposure concentration.

Request for the full study report

You must submit the full study report which includes:

- a complete rationale of test design and
- interpretation of the results
- access to all information available in the full study report, such as implemented method, raw data collected, interpretations and calculations, consideration of uncertainties, argumentation, etc.

This will enable the evaluating MSCA to fully and independently assess all the information

provided, including the statistical analysis, and to efficiently clarify the potential hazard for the PBT/vPvB properties for the Substance.

c) Alternative approaches and how the request is appropriate to meet its objective

The request for the Fish Early Life Stage Toxicity Test with the constituent Type A n=1 of the Substance is:

- Appropriate, because the test is suitable and necessary to obtain information which will allow clarifying whether the constituent of the Substance fulfils the REACH Annex XIII T criteria for long-term aquatic toxicity;
- The least onerous measure, because there is no equally suitable alternative methodology available, as a second step of aquatic toxicity testing, to obtain the information that would clarify the potential hazard.

2.6 Consideration of time needed to perform the requested studies

In your comments on the draft decision, you requested an extension of the timeline to 42 months to determine the water solubility (Request A.1) and perform the simulation study (Request A.2). You sought to justify this request due to the following:

(i.) Identification of suitable test laboratories with sufficient capacity;
(ii.) Constituent synthesis and radiolabelling; and
(iii.) Development of adapted analytical methods.

ECHA has considered the above and notes the following:

(i.) The standard 6-month timeline has been exceptionally extended for Request A.1 by an additional 6 months, to take into account the current longer lead times in contract research organisations (CRO's).
(ii.) Agrees that additional time may be needed, and has added 12 months for the synthesis and radiolabelling of the constituent Type A n=1.
(iii.) The time needed for analytical method development is already included within the standard timelines for water solubility and simulation studies. Since you have not provided any documentary evidence to support your justification as to why additional time is necessary, ECHA has not further amended the standard timelines on this basis.

Therefore, ECHA has extended the deadline to perform the water solubility study from 6 to 24 months. Consequently, the sequential deadlines for the other requests were amended to 42, 51, and 63 months, respectively.

3. References relevant to the requests (which are not included in the registration dossier)

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Appendix B: Procedure

This decision does not imply that the information you submitted in your registration dossier(s) are in compliance with the REACH requirements. ECHA may still initiate a compliance check on your dossiers.

12-month follow-up evaluation

- Due to initial grounds of concern for PBT/vPvB, the Member State Committee agreed to include the Substance (EC No 271-867-2, CAS RN 68610-51-5) in the Community rolling action plan (CoRAP) to be evaluated in 2016. Spain is the competent authority ('the evaluating MSCA') appointed to carry out the evaluation.

- In accordance with Article 46(3) of REACH, the evaluating MSCA carried out its evaluation based on the information in the registration dossier(s) you submitted on the Substance on 27 May 2021 subsequent to a decision dated 11 April 2018, and on other relevant and available information.

- The evaluating MSCA completed its follow-up evaluation considering that further information is required to clarify the following concerns: PBT/vPvB

- Therefore, it submitted a draft decision (Article 46(3) of REACH) to ECHA on 07 April 2022.

Decision making

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

The decision making followed the procedure of Articles 50 and 52 of REACH as described below.

(i) Registrant(s)' commenting phase

ECHA received your comments and forwarded them to the evaluating MSCA.

The evaluating MSCA took your comments into account (see Appendix A). The request(s) and the deadline were amended as explained in Section 2.6.

(ii) Proposals for amendment by other MSCAs and ECHA and referral to the Member State Committee

The evaluating MSCA notified the draft decision to the competent authorities of the other Member States and ECHA for proposal(s) for amendment.

Subsequently, the evaluating MSCA received proposals for amendment to the draft decision and modified the draft decision (see Appendix A).

ECHA referred the draft decision, together with your comments, to the Member State Committee.

ECHA invited you to comment on the proposed amendments. Your provided comments were not considered at this stage as they were outside the scope of the proposals for amendment and thus outside the scope of Article 52(2) and Article 51(5). This is because these comments reiterated your previous comments on selection of constituent Type A (n=1), assessment of bioaccumulation of constituents Type A (n=1) and Type B (n=1),

and the deadlines for submission of the requested information. These topics were not subject to a proposal for amendment.

(iii) MSC agreement seeking stage

The Member State Committee reached a unanimous agreement in its MSC-80 written procedure and ECHA took the decision according to Article 52(2) and Article 51(6) of REACH.

After the deadline set in this decision has passed, the evaluating MSCA will review the information you will have submitted and will evaluate whether further information is still needed to clarify the potential risk, according to Article 46(3) of REACH. Therefore, a subsequent evaluation of the Substance may still be initiated after the present substance evaluation is concluded.

Appendix C: Technical Guidance to follow when conducting new tests for REACH purposes

Test methods, GLP requirements and reporting

Under Article 13(3) of REACH, all new data generated as a result of this decision must be conducted according to the test methods laid down in a European Commission Regulation or to international test methods recognised by the Commission or ECHA as being appropriate.

Under Article 13(4) of REACH, ecotoxicological and toxicological tests and analyses must be carried out according to the GLP principles (Directive 2004/10/EC) or other international standards recognised by the Commission or ECHA.

Under Article 10(a)(vi) and (vii) of REACH, all new data generated as a result of this decision must be reported as study summaries, or as robust study summaries, if required under Annex I of REACH. See ECHA Practical Guide on How to report robust study summaries[4].

Test material

Before generating new data, you must agree within the joint submission on the chemical composition of the material to be tested (Test Material) which must be relevant for all the registrants of the Substance.

1. *Selection of the Test material(s)*

   The Test material used to generate the new data is specific constituent (Type A n=1) of the Substance and the requirements regarding the test material, as described in Appendix A in this decision, must be followed, taking into account also the following:
   - the variation in compositions reported by all members of the joint submission,
   - the boundary composition(s) of the Substance,
   - the impact of each constituent/ impurity on the test results for the endpoint to be assessed.

2. *Information on the Test Material needed in the updated dossier*

   a) You must report the composition of the Test Material selected for each study, under the 'Test material information' section, for each respective endpoint study record in IUCLID.
   b) The reported composition must include all constituents of each Test Material and their concentration values.

This information is needed to assess whether the Test Material is relevant for the Substance and whether it is suitable for use by all members of the joint submission.

Technical instructions on how to report the above is available in the manual "How to prepare registration and PPORD dossiers"[5].

[4] https://echa.europa.eu/practical-guides
[5] https://echa.europa.eu/manuals