~~Confidential~~

Helsinki, 24 November 2022

Addressees
Registrant(s) of Joint subm. TDEC as listed in Appendix 3 of this decision

Date of submission of the dossier subject to this decision
04/10/2018

Registered substance subject to this decision ("the Substance")
Substance name: Tetrakis(diethyldithiocarbamato-S,S')tellurium
EC number: 244-121-9

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

DECISION ON A COMPLIANCE CHECK

Under Article 41 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below, by the deadline of ***31 August 2026***.

Requested information must be generated using the Substance unless otherwise specified.

Information required from all the Registrants subject to Annex VII of REACH

1. Partition coefficient n-octanol/water (Annex VII, Section 7.8.; using an appropriate test method);

2. Skin sensitisation (Annex VII, Section 8.3.); test methods:

   i. In vitro/in chemico skin sensitisation information on molecular interaction with skin proteins and inflammatory response in keratinocytes and activation of dendritic cells (OECD TG 442C and OECD TG 442D and EU B.71/OECD TG 442E); and

   ii. Only in case no conclusion on the skin sensitisation potency can be made for the Substance based on the newly generated in vitro/in chemico data, in vivo skin sensitisation study must be performed and the murine local lymph node assay (EU Method B.42/OECD TG 429) is considered as the appropriate study for the potency estimation;

3. Long-term toxicity testing on aquatic invertebrates (triggered by Annex VII, Section 9.1.1., column 2; test method: EU C.20./OECD TG 211).

Information required from all the Registrants subject to Annex VIII of REACH

4. Hydrolysis as a function of pH (Annex VIII, Section 9.2.2.1.; test method: EU C.7./OECD TG 111).;

5. Long-term toxicity testing on fish (triggered by Annex VIII, Section 9.1.3., column 2; test method: EU C.47./OECD TG 210);

6. Simulation testing on ultimate degradation in surface water (triggered by Annex VIII, Section 9.2.; test method: EU C.25./OECD TG 309) at a temperature of 12°C. Non-extractable residues (NER) must be quantified and a scientific justification of the selected extraction procedures and solvents must be provided;

7. Soil simulation testing (triggered by Annex VIII, Section 9.2.; test method: EU C.23./OECD TG 307) at a temperature of 12°C. Non-extractable residues (NER) must be quantified and a scientific justification of the selected extraction procedures and solvents must be provided;

8. Sediment simulation testing (triggered by Annex VIII, Section 9.2.; test method: EU C.24./OECD TG 308) at a temperature of 12°C. Non-extractable residues (NER) must be quantified and a scientific justification of the selected extraction procedures and solvents must be provided;

9. Identification of degradation products (triggered by Annex VIII, Section 9.2; test method: EU C.25./OECD TG 309, EU C.23./OECD TG 307 or EU C.24./OECD TG 308).

The reasons for the decision are explained in Appendix 1.

Information required depends on your tonnage band

You must provide the information listed above for all REACH Annexes applicable to you in accordance with Articles 10(a) and 12(1) of REACH. The addressees of the decision and their corresponding information requirements based on registered tonnage band are listed in Appendix 3.

You are only required to share the costs of information that you must submit to fulfil your information requirements.

How to comply with your information requirements

To comply with your information requirements, you must submit the information requested by this decision in an updated registration dossier by the deadline indicated above. You must also **update the chemical safety report,** where relevant, including any changes to classification and labelling, based on the newly generated information.

You must follow the general requirements for testing and reporting new tests under REACH, see Appendix 4. In addition, the studies relating to biodegradation and bioaccumulation are necessary for the PBT assessment. However, to determine the testing needed to reach the conclusion on the persistency and bioaccumulation of the Substance you should consider the sequence in which these tests are performed and other conditions described in this Appendix.

Appeal

This decision, when adopted under Article 51 of REACH, 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.

~~Confidential~~

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

Appendix 1: Reasons for the decision
Appendix 2: Procedure
Appendix 3: Addressees of the decision and their individual information requirements
Appendix 4: Conducting and reporting new tests under REACH

[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 for the decision

Contents

Reasons related to the information under Annex VII of REACH

1. Partition coefficient n-octanol/water

1 Partition coefficient n-octanol/water is a standard information requirement in Annex VII to the REACH Regulation.

1.1. *Information provided*

2 You have provided an estimated Log Kow of 4.389 based on a prediction from the QSAR KOWWIN.

3 You state that the results are 'derived from a valid (Q)SAR model, but not (completely) falling into its applicability domain'.

1.2. *Assessment of the information provided*

4 We have assessed this information and identified the following issue(s): the substance is outside the applicability domain of the model.

5 Under the Guidance on IRs & CSA Section R.6.1.5.3., a substance must fall within the applicability domain specified by the model developer.

6 The applicability domain of the model includes the following requirements:

- the maximum number of occurrences of the -S- fragment should not exceed two (2) as the maximum number of -S- fragments in the training and validation set of the KOWWIN QSAR is two;
- the substance should not contain structural fragments or elements unknown to the KOWWIN QSAR e.g. fragments/elements not represented in the training set of the model.

7 The Substance used as input for the prediction has the following properties related to the estimation of applicability domain:

- the Substance has four (4) -S- fragments and therefore exceeds the maximum number of occurrences of the -S- fragment in the training and validation set of the KOWWIN QSAR and;
- the Substance contains the structural fragment N-C(=S)-S and an element (Te) which are unknown to the QSAR i.e. not represented in the training set of the model.

8 The Substance used as input for the prediction contains fragments that exceed the maximum number defined in the applicability domain of the KOWWIN QSAR, as well as fragments and an element (Te) not represented in the training set of the QSAR. Therefore the Substance is outside the applicability domain and the prediction for Log Kow is not reliable.

9 You acknowledge in the dossier, and in the QPRF, that the Substance does not fit within the applicability domain of the KOWWIN QSAR.

10 Therefore, you have not demonstrated that the Substance falls within the applicability domain of the model.

11 On this basis the information requirement is not fulfilled. Consequently there is an information gap and it is necessary to provide information for this endpoint.

12 In your comments on the draft decision, you agree to conduct the required study.

13 Guidance for determining appropriate test methods for the partition coefficient n-octanol/water is available in the Guidance on IRs & CSA, Section R.7.1.8.

2. Skin sensitisation

14 Skin sensitisation is an information requirement under Annex VII to REACH (Section 8.3.). Under Section 8.3., Column 1, the registrants must submit information allowing (1) A) a conclusion whether the substance is a skin sensitiser and B) whether it can be presumed to have the potential to produce significant sensitisation in humans (Cat. 1A), and (2) risk assessment, where required.

2.1. *Information provided*

15 You have provided a Buehler test in guinea pigs ([redacted], 1986) with the Substance.

2.2. *Assessment of the information provided*

16 We have assessed this information and identified the following issue(s):

2.2.1. Non-compliant study

17 To be considered compliant and enable concluding whether the Substance causes skin sensitisation, a study has to meet the requirements of the EU Method B.6/OECD TG 406. The following key parameters of this test guideline include:

a. Dose level selection rationale;
b. The induction concentration should be the highest causing mild irritation to the skin and the challenge dose should be the highest non-irritation concentration (OECD TG 406, paragraph 27);
c. Appropriate number of animals (20 in the treated groups and 10 in the control group);
d. Positive and negative controls to establish the sensitivity and reliability of the experimental technique (OECD TG 406, paragraph 11).

18 However, ECHA notes that for the provided study:

a. No dose level selection rationale was provided;
b. The concentration used for induction did not cause mild irritation;
c. Only 10 animals/dose were used;
d. Positive and negative control groups were not included in the study and there is no other information available to confirm the sensitivity and reliability of the experimental technique.

19 On this basis, the information requirement is not fulfilled.

2.2.2. No assessment of potency

20 To be considered compliant and enable a conclusion in cases where the substance is considered to cause skin sensitisation, the information provided must also allow a conclusion whether it can be presumed to have the potential to produce significant sensitisation in humans (Cat. 1A).

21 As the currently available data does not allow to conclude whether the Substance causes skin sensitisation (see section 2.2.1. above), this condition cannot be assessed.

22 On this basis, the information requirement is not fulfilled.

2.3. *Specification of the study design*

23 To fulfil the information requirement for the Substance, information on molecular interaction with skin proteins and inflammatory response in keratinocytes and activation of dendritic cells (OECD TG 442C and OECD TG 442D and EU B.71/OECD TG 442E) must be provided. Furthermore, an appropriate risk assessment is required if a classification of the Substance as a skin sensitiser (Cat 1A or 1B) is warranted.

24 In case no conclusion on the skin sensitisation potency can be made for the Substance based on the newly generated in vitro/in chemico data, in vivo skin sensitisation study must be performed and the murine local lymph node assay (EU Method B.42/OECD TG 429) is considered as the appropriate study for the potency estimation.

2.4. *Information provided in your comments on the draft decision*

25 In your comments on the draft decision you recognise that the information included in your dossier is not according to the current standards. You indicate that as a pre-cautionary action you will self-classify the Substance as skin sensitiser category 1 based on the properties from the structurally similar substance Zinc bis(diethyldithiocarbamate) (ZDEC, CAS 14324-55-1), which is classified as Skin Sens. Cat. 1.

26 In the comments to the draft decision you express your intentions to use information from a structurally related substance to derive the properties of the Substance, i.e. your intentions to submit an adaptation of the information requirement according to Annex XI, Section 1.5 instead of conducting the requested study. ECHA understands that you consider that such an adaptation would constitute a worst-case approach leading to the classification of the Substance as skin sensitiser category 1.

27 Based on the information provided in the comments, ECHA cannot assess whether your adaptation fulfils the requirements of Section 1.5 of Annex XI to the REACH Regulation as you have not provided further endpoint-specific documentation of your planned adaptation.

28 Therefore, the data gap persists and you remain responsible for complying with this decision by the set deadline.

3. Long-term toxicity testing on aquatic invertebrates

29 Short-term toxicity testing on aquatic invertebrates is an information requirement under Column 1 of Annex VII to REACH (Section 9.1.1.). However, long-term toxicity testing on aquatic invertebrates must be considered (Section 9.1.1., Column 2) if the substance is poorly water soluble.

3.1. *Information provided*

30 You have provided an OECD TG 202 study ([redacted] 2018) but no information on long-term toxicity on aquatic invertebrates for the Substance.

3.2. *Assessment of the information provided*

31 We have assessed this information and identified the following issue:

32 Poorly water soluble substances require longer time to reach steady-state conditions. As a result, the short-term tests does not give a true measure of toxicity for this type of substances and the long-term test is required. A substance is regarded as poorly water soluble if, for instance, it has a water solubility below 1 mg/L or below the detection limit of the analytical method of the test material (Guidance on IRs and CSA, Section R.7.8.5).

33 In the provided OECD TG 105 study ([redacted] 2018), the saturation concentration of the Substance in water was determined to be 0.634 mg/L.

34 Therefore, the Substance is poorly water soluble and information on long-term toxicity on aquatic invertebrates must be provided.

35 In your comments on the draft decision, you agree to conduct the required study.

3.3. *Study design and test specifications*

36 The Substance is difficult to test due to the low water solubility (0.634 mg/L) and rapid hydrolysis (e.g. DT50 at pH 7 and 20°C is 54 mins). OECD TG 211 specifies that, for difficult to test substances, you must consider the approach described in OECD GD 23 or other approaches, if more appropriate for your substance. In all cases, the approach selected must be justified and documented. Due to the properties of Substance, it may be difficult to achieve and maintain the desired exposure concentrations. Therefore, you must monitor the test concentration(s) of the Substance throughout the exposure duration and report the results. If it is not possible to demonstrate the stability of exposure concentrations (i.e. measured concentration(s) not within 80-120% of the nominal concentration(s)), you must express the effect concentration based on measured values as described in OECD TG 211. In case a dose-response relationship cannot be established (no observed effects), you must demonstrate that the approach used to prepare test solutions was adequate to maximise the concentration of the Substance in the test solutions.

Reasons related to the information under Annex VIII of REACH

4. Hydrolysis as a function of pH

37 Hydrolysis as a function of pH is an information requirement under Column 1 of Annex VIII to REACH (Section 9.2.2.1). Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

4.1. *Information provided*

38 You have provided a hydrolysis study according to the OECD TG 111 ([redacted] 2018) on the Substance. This study indicates that the Substance rapidly hydrolyses (at 20°C the DT50s were 13 mins and 54 mins at pH 4 and 7, respectively). The hydrolysis rate increased with decreasing pH and increasing temperature (e.g. at 50°C and pH 4 you state that the DT50 could not be determined due to the very rapid hydrolysis rate).

39 You have provided no information on the identity of the hydrolysis products.

4.2. *Assessment of the information provided*

40 We have assessed this information and identified the following issue:

41 The Guidance on IRs & CSA Section R.11.4.1.1 states that hydrolysis products should be identified in accordance with the recommendations contained in the test guidelines (e.g. OECD TG 111). The OECD TG 111 requires that major hydrolysis products (at least those representing > 10% of the applied dose) must be identified by appropriate analytical methods.

42 In the provided OECD TG 111 study on the Substance ([redacted] 2018), you have provided no information on the identity of the hydrolysis products.

43 As the information provided does not contain information on the identity of the hydrolysis products for the Substance as prescribed by the OECD TG 111, it is not adequate to fulfil the information requirement. Consequently there is an information gap and it is necessary to provide information for this endpoint.

44 The identity of the hydrolysis products as well as their rates of formation is required for the hazard assessment for the Substance. Therefore, hydrolysis testing (including the identification of the hydrolysis products and their rates of formation) should be conducted.Study design and test specifications

45 To fulfil the information requirement for the Substance, information on the identity of the hydrolysis products as well as their rates of formation must be provided (OECD TG 111).

4.3. *Information provided in your comments on the draft decision*

46 In your comments on the draft decision you have provided the following:

47 You do not agree to perform the requested study. Instead, you indicate that you intend to adapt this information requirement by using a read-across approach according to Annex XI, Section 1.5, of the REACH Regulation and you provide the following information:

(i) Description of the study design and results from a hydrolysis study according to OECD TG 111 for zinc bis(diethyldithiocarbamate) (ZDEC, Cas# 14324-55-1).
(ii) Read-across justification document in the Annex.

48 You provide the following reasoning for the prediction of this information requirement: "TDEC hydrolyses similarly to ZDEC, and its hydrolysis products are similar to the hydrolysis products of analogue ZDEC.".

49 ECHA understands that you predict the properties of the Substance using a read-across hypothesis which is based on the formation of common (bio)transformation products. The properties of your Substance are predicted to be quantitatively equal to those of the source substance.

50 Regarding the read across using an analogue substance (ZDEC) to identify the hydrolysis products of the Substance:

51 Annex XI, Section 1.5 requires that whenever read-across is used adequate and reliable documentation of the applied method must be provided. Such documentation must include an explanation why the properties of the Substance may be predicted from other substances in the group, i.e. a read-across hypothesis. This hypothesis should be based on recognition of the structural similarities and differences between the substances (Guidance on IRs and CSA, Section R.6.).It should explain why the differences in the chemical structures should not influence the environmental fate properties or should do so in a regular pattern, taking into account that variations in chemical structure can affect environmental fate of substances (Guidance on IRs and CSA, Section R.6.2.1.3).

52 Your read-across hypothesis is based on the transformation of the Substance and of the source substance(s) to common compound(s). In this context, information characterising the rate and extent of the transformation of the Substance and of the source substance(s) is necessary to confirm the formation of the proposed common transformation products and to assess the impact of the exposure to the parent compounds.

53 Supporting information must include information on the formation of common compounds, and consideration of the potential for non-common compounds to be formed.

54 Your read-across hypothesis is based on structural similarities in the organic moiety of the source substance. You consider that this element is a sufficient basis for predicting the hydrolysis properties of the Substance, including the identity of all the hydrolysis products.

55 Structural similarity in the organic moiety of the source substance alone does not necessarily lead to predictable or similar hydrolysis properties, particularly in regard to the identity of the hydrolysis products.

56 The source substance contains Zinc (Zn) whereas the Substance contains Tellurium (Te). You do not address this key difference between the source substance and the Substance in your read across, or the expected impact on the identity of the hydrolysis products.

57 Based on the results of the hydrolysis study on ZDEC (i) you state that the hydrolysis products from ZDEC and the Substance will be the same. The only identified hydrolysis product from study on ZDEC was carbon disulphide (CS_2). ECHA acknowledges that one of the final hydrolysis products from the Substance could be CS_2. However, CS_2 is not the only hydrolysis product that is expected to be formed. The Substance contains tellurium which exists in varying oxidation states both in vivo and in the environment. The hydrolysis study on ZDEC (i) provides no information on the identity or rate of formation for tellurium-containing hydrolysis products. In your read-across justification document, you do not address the potential for hydrolysis products containing tellurium to be formed, or their potential oxidation states. You do not consider that tellurium-containing hydrolysis products of potential (eco)toxicity concern may be formed and that information on their identity, rates of formation, and half-lives are important in the hazard assessment of the Substance.

58 As explained above, you have not established that relevant properties of the Substance can be predicted from data on the analogue substances. Therefore, your adaptation does not

comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and your read-across approach is rejected.

59 Therefore, the data gap persists and you remain responsible for complying with this decision by the set deadline.

5. Long-term toxicity testing on fish

60 Short-term toxicity testing on fish is an information requirement under Column 1 of Annex VIII to REACH (Section 9.1.3.). However, long-term toxicity testing on fish must be considered (Section 9.1.3., Column 2) if the substance is poorly water soluble.

5.1. *Information provided*

61 You have provided an OECD TG 203 study ([redacted] 2018) but no information on long-term toxicity on fish for the Substance.Assessment of the information provided

62 We have assessed this information and identified the following issue:

63 Poorly water soluble substances require longer time to reach steady-state conditions. As a result, the short-term tests does not give a true measure of toxicity for this type of substances and the long-term test is required. A substance is regarded as poorly water soluble if, for instance, it has a water solubility below 1 mg/L or below the detection limit of the analytical method of the test material (Guidance on IRs and CSA, Section R.7.8.5).

64 As already explained under Section 3, the Substance is poorly water soluble and information on long-term toxicity on fish must be provided.

5.1.1. Information provided in your comments on the draft decision

65 In your comments on the draft decision you propose to conduct the long-term toxicity to aquatic invertebrates OECD TG 211 study (request 3) 'before deciding if an OECD TG 210 study is necessary'. You do not agree to perform the long-term toxicity to fish study as requested in the draft decision due to the following reasons:

66 'The available aquatic toxicity studies on three trophic levels (fish, invertebrate and algae) show that fish is the least sensitive species and aquatic invertebrate is the most sensitive species….. We acknowledge that the low water solubility of TDEC may impact the results of the species sensitivity. If the OECD TG 211 study shows that aquatic invertebrate is more sensitive than algae (ErC10 = 34 µg/L, OECD TG 201), the sensitivity of chronic exposure will be consistent with the acute exposure results. Then the long-term toxicity of TDEC to fish can be waived based on the test on invertebrates and algae.'

67 Furthermore, you state that 'This is also in line with animal welfare by reducing the number of fish used for testing.'

68 ECHA has assessed the information provided in the comments and identified the following issue(s):

69 A registrant may only adapt this information requirement based on the general rules set out in Annex XI.

70 Your justification to omit the study does not refer to any of the adaptation possibilities in Annex XI. Therefore, the arguments provided in your comments are not appropriate to adapt the information requirement. Furthermore, minimisation of vertebrate animal testing is not on its own a legal ground for adaptation under the general rules of Annex XI.You refer to differences in species sensitivies among fish and daphnids based on results of short-term studies to justify why long-term daphnia should be conducted first and why long-term fish might not be needed. However, as already explained above short-term studies cannot

be used to conclude on hazards and long-term studies are needed. In conclusion, in your comments you have not provided any acceptable reason why long-term toxicity to fish should be omitted or conducted conditionally to long-term toxicity to aquatic invertebrates (Request 3). Since there is a data gap for both endpoints, ECHA requests that both studies are conducted.

5.2. *Study design and test specifications*

71 To fulfil the information requirement for the Substance, the Fish, Early-life Stage Toxicity Test (test method OECD TG 210) is the most appropriate (Guidance on IRs and CSA, Section R.7.8.2.).

72 The OECD TG 210 specifies that, for difficult to test substances, the OECD GD 23 must be followed. As already explained above, the Substance is difficult to test. Therefore, you must fulfil the requirements described in 'Study design and test specifications' in Section 3.

6. Simulation testing on ultimate degradation in surface water

73 Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., Column 2).

74 This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (Guidance on IRs and CSA, Section R.11.4.). This is the case if the Substance itself or any of its constituent or impurity present in concentration ≥ 0.1% (w/w) or relevant transformation/degradation product meets the following criteria:

- it is potentially persistent or very persistent (P/vP) as:
  - it is not readily biodegradable (*i.e.* <60% degradation in an OECD 301B), and;
- it is potentially bioaccumulative or very bioaccumulative (B/vB) as:
  - it has a high potential to partition to lipid storage (*e.g.* log K_{ow} > 4.5);
- it meets the T criteria set in Annex XIII: NOEC or EC_{10} < 0.01 mg/L or classification as carc. 1A or 1B, muta. 1A or 1B, repro. 1A, 1B or 2, or STOT RE 1 or 2.

6.1. *Information provided*

75 Your registration dossier provides the following:

- The Substance is not readily biodegradable (6% degradation after 28 days in OECD TG 301B);
- The Substance has a high potential to partition to lipid storage. As explained in Section 1, the provided Log K_{ow} of 4.39 based on KOWWIN QSAR prediction is not reliable. You state that the Substance has '*high lipophilicity*' in Section 5.1.3 of the CSR and in Section 7.1 of IUCLID.

76 Furthermore, the information in your dossier is currently incompliant and therefore:

- it is not possible to conclude on the bioaccumulation potential of the Substance (see Request in Section 1 of this decision), and

- it is not possible to conclude on the toxicity of the Substance (see Requests in Sections 3 and 5 of this decision).

77 Under section 2.3 of your IUCLID dossier ('PBT assessment'), you conclude that the Substance is not B/vB. In support of your conclusion you provide the following statement: 'The test substance is considered not bioaccumulative as the substance has a log Kow of ≤4.5 and may therefore be considered to be "not B/vB".'

78 However, as explained in Section 1 the reported Log Kow value of 4.39 is not reliable and it cannot be excluded that the Log Kow would not exceed 4.5. In addition, you state in your dossier that the Substance has high lipophilicity. Therefore, high potential for bioaccumulation cannot be excluded based on available information.

79 Therefore, the additional information from your PBT assessment is not adequate to conclude that the Substance is not a potential PBT/vPvB substance.

80 Based on the above, the available information on the Substance indicates that it is a potential PBT/vPvB substance.

81 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation.

6.1.1. Information provided in your comments on the draft decision

82 In your comments on the draft decision you acknowledge that the Substance is not readily biodegradable. You also acknowledge that the current partition coefficient (Log Kow) information is unreliable, hence it is currently not possible to conclude if the substance is a potential PBT/vPvB substance nor if it is highly adsorptive.

83 Therefore, you propose the following testing strategy in order to conclude on the PBT/vPvB properties of the Substance:

84 i) You propose to conduct the partition coefficient testing first (request 1) and only if the Log Kow is >4.5 you will consider simulation testing.

85 ii) You also consider that if the Log Kow is >4.5, soil and sediment are more relevant compartments than water for simulation testing, due to high potential to adsorb to soil and sediment (especially considering the low water solubility). You further refer to the rapid hydrolysis of the Substance. We understand from your comments that you consider to omit the surface water study if the Log Kow is found to be >4.5.

86 We have assessed the information provided in your comments on the draft decision and identified the following issues:

87 i) In regard to the proposed testing strategy based on the results of the partition coefficient testing, and the subsequent sequence of simulation tests:

88 If the partition coefficient testing demonstrates a lack of bioaacumulation concern (i.e. Log Kow <4.5) then the CSA would not require further simulation testing. However, since reliable data on Log Kow are not currently available your proposed strategy relies essentially on data that has yet to be generated, therefore it cannot yet contribute to conclusions on the compliance of the registration dossier.

89 ii) In regard to omitting the surface water study if LogKow>4.5

- Guidance on IRs and CSA, Section R.11.4.1.1.1 states that the OECD TG 309 is the preferred test to start persistency assessment and if another test is selected for further testing, this should be justified, based on the following: The aquatic compartment is not considered relevant at all, and there are compartment specific concerns for the sediment and soil compartments, including indications from

available data (e.g. literature) suggesting that persistence is likely to occur in a different environmental compartment (i.e. in soil or sediment).

90 You claim in your comments on the draft decision that the surface water simulation test could be omitted because soil and sediment are more appropriate compartments for simulation testing based on the following:

- the Substance is expected to distribute to soil and sediment since it has high adsorption potential (as indicated by low water solubility), and is hydrolysable.

91 We have assessed your comments and note the following issues: As stated in Appendix 2.1 of this decision you may decide on the sequence of simulation degradation testing considering the intrinsic properties of the Substance, and its identified uses and release patterns. You may therefore choose to conduct simulation studies starting with the worst case scenarios for persistence, with appropriate justifications.

92 In your comments on the draft decision you propose to omit simulation in water since you consider water is not a relevant compartment only based on intrinsic properties of the Substance (i.e. high adsorption potential and hydrolysis), without providing any evidence that water would not be a relevant compartment based on uses and release patterns and based on water not being worst-case for P/vP.

93 Regarding simulation in surface water; the aquatic compartment is considered to be a relevant environmental compartment since, by default, the water compartment receives significant amount of emissions directly or indirectly, and transports/distributes the substance through e.g. deposition and run-off (unless based on the fate and release(s) of the substance, it is considered that the water compartment is not a relevant environmental compartment at all). Once entering water, a substance may stay there for very long time and be spread over long distances before it reaches other environmental compartments (via environmental transport, partitioning and distribution processes) such as sediments or (via air) the soil compartment.

94 In addition, the Substance is adsorptive and particularly for lower water solubility substances which tend to be adsorptive, the OECD TG 309 (with a default concentration of suspended solids of 15 mg dw/L) minimizes potential non-extractable residues (NER) formation. If NER is formed at significant levels in the OECD TGs 307 and 308 studies, this can be difficult to interpret and compare with degradation half-lives criteria of Annex XIII to the REACH Regulation (Guidance on IRs and CSA, Section R.11.4.1.1.1).

95 For these reasons the OECD TG 309 is relevant for the Substance and you have not demonstrated in your comments on the draft decision that the aquatic compartment is not a relevant compartment at all.

96 Therefore, the data gap persists and you remain responsible for complying with this decision by the set deadline.

6.2. *Study design and test specifications*

97 Simulation degradation studies must include two types of investigations (Guidance on IRs and CSA, Section R.7.9.4.1.):

1) a degradation pathway study where transformation/degradation products are quantified and, if relevant, are identified, and

2) a kinetic study where the degradation rate constants (and degradation half-lives) of the parent substance and of relevant transformation/degradation products are experimentally determined.

98 You must perform the test, by following the pelagic test option with natural surface water containing approximately 15 mg dw/L of suspended solids (acceptable concentration between 10 and 20 mg dw/L) (Guidance on IRs and CSA, Section R.11.4.1.1.3.).

99 The required test temperature is 12°C, which corresponds to the average environmental temperature for the EU (Guidance on IRs and CSA, Table R.16-8) and is in line with the applicable test conditions of the OECD TG 309.

100 As specified in Guidance on IRs and CSA, Section R.7.9.4.1., the organic carbon (OC) concentration in surface water simulation tests is typically 2 to 3 orders of magnitude higher than the test material concentration and the formation of non-extractable residues (NERs) may be significant in surface water tests. Therefore, non-extractable residues (NER) must be quantified. 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) (Guidance on IRs and CSA, Section R.11.4.1.1.3.). Further recommendations may be found in the background note on options to address non-extractable residues in regulatory persistence assessment available on the ECHA website.

101 Relevant transformation/degradation products are at least those detected at ≥ 10% of the applied dose at any sampling time or those that are continuously increasing during the study even if their concentrations do not exceed 10% of the applied dose, as this may indicate persistence (OECD TG 309; Guidance on IRs and CSA, Section R.11.4.1.).

7. Soil simulation testing

102 Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., Column 2).

103 This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (Guidance on IRs and CSA, Section R.11.4.).

104 As already explained in Section 6, the Substance is a potential PBT/vPvB substance.

105 Further, the Substance has a low water solubility (0.634 mg/L), and a high potential to adsorb to soil cannot be excluded. As explained in Section 1, the provided Log Kow of 4.39 is unreliable. Therefore it cannot be excluded that the Log Kow of the Substance is >4.5 indicating a high potential to adsorb to soil.

106 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation. Based on the adsorptive properties of the Substance, soil represents a relevant environmental compartment.

7.1.1. Information provided in your comments on the draft decision

107 In your comments on the draft decision you acknowledge that the Substance is not readily biodegradable. You also acknowledge that the current partition coefficient (Log Kow) information is unreliable, hence it is currently not possible to conclude if the Substance is a potential PBT/vPvB substance nor if it is highly adsorptive.

108 Therefore, you propose the following testing strategy in order to conclude on the PBT/vPvB of the Substance:

109 i) You propose to conduct the partition coefficient testing first (request 1) and only if the Log Kow is >4.5 you will consider simulation testing.

110 ii) You also indicate that you consider the sediment and soil compartments relevant based on properties of the Substance including high adsorptivity, low water solubility, and rapid hydrolysis. However, you propose a testing strategy before considering simulation testing in different compartments and you indicate that you would conduct the sediment study first. You consider that if the Substance is concluded to be persistent in this test, this information would be sufficient to conclude the Substance is P/vP and the soil study would not be necessary. You indicate that you would conduct a bioaccumulation study rather than the soil simulation study if the Substance is found to be persistent in the sediment simulation study.

111 We have assessed the information provided in your comments on the draft decision and identified the following issues:

112 i) In regard to the proposed testing strategy based on the results of the partition coefficient testing

113 As explained in Section 6.1, if the partition coefficient testing demonstrates a lack of bioaacumulation concern (i.e. Log Kow <4.5) then the CSA would not require further simulation testing. However, since reliable data on Log Kow are not currently available your proposed strategy relies essentially on data that has yet to be generated, therefore it cannot yet contribute to conclusions on the compliance of the registration dossier.

114 ii) In regard to omitting the soil study if the sediment simulation study (request 8) shows P/vP concern

115 Appropriate data needs to be available to conclude on the P/vP-assessment with a conclusion "not P/vP" on all three (five) compartments: water (marine water), sediment (marine sediment) and soil. If a conclusion "P" or "vP" is reached for one compartment, no further testing or assessment of persistence of other environmental compartments is normally necessary (Guidance on IRs and CSA, Section R.11.4.1.1.1).

116 In your comments you propose to initiate simulation testing on sediment (request 8) and to omit simulation in soil if the Substance is concluded P or vP.

117 As indicated in Appendix 2.1, you may choose the sequence of simulation testing with appropriate justifications based on intrinsic properties, uses, releases, and the compartment considered most likely to provide a worse-case assessment of persistence. Since the Substance is a potential PBT or vPvB substance and currently no conclusion can be made on B and T properties of the Substance (as explained in Section 6.1), the sequence of simulation testing can only cease if there is a conclusion of vP in a previous test.

118 As this approach relies on data yet to be generated, ECHA cannot make a conclusion on the need to perform the requested test in order to conclude on P/vP.ECHA refers you to Appendix 2.1 for guidance on the recommended sequence of testing for PBT/vPvB assessment. The deadline set in this decision allows sufficient time for sequential testing.

119 Therefore, the data gap persists and you remain responsible for complying with this decision by the set deadline.

7.2. *Study design and test specifications*

120 Simulation degradation studies must include two types of investigations (Guidance on IRs and CSA, Section R.7.9.4.1.):

1) a degradation pathway study where transformation/degradation products are quantified and, if relevant, are identified, and

2) a kinetic study where the degradation rate constants (and degradation half-lives) of the parent substance and of relevant transformation/degradation products are experimentally determined.

121 In accordance with the specifications of the OECD TG 307, you must perform the test using at least four soils representing a range of relevant soils (i.e. varying in their organic content, pH, clay content and microbial biomass).

122 The required test temperature is 12°C, which corresponds to the average environmental temperature for the EU (Guidance on IRs and CSA, Table R.16-8) and is in line with the applicable test conditions of the OECD TG 307.

123 In accordance with the specifications of the OECD TG 307, non-extractable residues (NER) must be quantified. The reporting of results must include a scientific justification of the used extraction procedures and solvents (Guidance on IRs and CSA, Section R.7.9.4.1.). 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) (Guidance on IRs and CSA, Section R.11.4.1.1.3.). Further recommendations may be found in the background note on options to address non-extractable residues in regulatory persistence assessment available on the ECHA website.

124 Relevant transformation/degradation products are at least those detected at ≥ 10% of the applied dose at any sampling time or those that are continuously increasing during the study even if their concentrations do not exceed 10% of the applied dose, as this may indicate persistence (OECD TG 307; Guidance on IRs and CSA, Section R.11.4.1.).

8. Sediment simulation testing

125 Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., Column 2).

126 This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (Guidance on IRs and CSA, Section R.11.4.).

127 As already explained in Section 6, the Substance is a potential PBT/vPvB substance.

128 Further, the Substance has a low water solubility (0.634 mg/L), and a high potential to adsorb to sediment cannot be excluded. As explained in Section 1, the provided Log Kow of 4.39 is unreliable. Therefore it cannot be excluded that the Log Kow of the Substance is >4.5 indicating a high potential to adsorb to sediment.

129 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation. Based on the adsorptive properties of the Substance, sediment represents a relevant environmental compartment.

8.1.1. Information provided in your comments on the draft decision

130 In your comments on the draft decision you acknowledge that the Substance is not readily biodegradable. You also acknowledge that the current partition coefficient (Log Kow) information is unreliable, hence it is currently not possible to conclude the Substance is a potential PBT/vPvB substance nor if it is highly adsorptive.

131 Therefore, you propose the following testing strategy in order to conclude on the PBT/vPvB properties of the Substance:

132 i) You propose to conduct the partition coefficient testing first (request 1) and only if the Log Kow is >4.5 you will consider simulation testing.

133 ii) You also indicate in your comments that you consider the sediment and soil compartments relevant based on properties of the Substance including high adsorptivity, low water solubility, and rapid hydrolysis. However, you propose a testing strategy before considering simulation testing in different compartments and you indicate that you would conduct the sediment study first.

134 We have assessed the information provided in your comments on the draft decision and identified the following issues:

135 i) In regard to the proposed testing strategy based on the results of the partition coefficient testing

136 As explained in Section 6.1.1, if the partition coefficient testing demonstrates a lack of bioaacumulation concern (i.e. Log Kow <4.5) then the CSA would not require further simulation testing. However, since reliable data on Log Kow are not currently available your proposed strategy relies essentially on data that has yet to be generated, therefore it cannot yet contribute to conclusions on the compliance of the registration dossier.

137 ii) In regard to starting the persistence testing with sediment

138 You may choose the sequence of testing with appropriate justifications. ECHA acknowledges your intention to start with simulation in sediment and points you to the comments in Section 6.1.1 and 7.1.1 with regards to your comments on simulation testing in other compartments. Note that Appendix 2.1 provides guidance on the recommended sequence of testing for PBT/vPvB assessment and the deadline set in this decision allows sufficient time for sequential testing.

139 Therefore, the data gap persists and you remain responsible for complying with this decision by the set deadline.

8.2. *Study design and test specifications*

140 Simulation degradation studies must include two types of investigations (Guidance on IRs and CSA, Section R.7.9.4.1.):

1) a degradation pathway study where transformation/degradation products are quantified and, if relevant, are identified, and

2) a kinetic study where the degradation rate constants (and degradation half-lives) of the parent substance and of relevant transformation/degradation products are experimentally determined.

141 In accordance with the specifications of the OECD TG 308, you must perform the test using two sediments. One sediment should have a high organic carbon content (2.5-7.5%) and a fine texture, the other sediment should have a low organic carbon content (0.5-2.5%) and a coarse texture. If the Substance may also reach marine waters, at least one of the water-sediment systems should be of marine origin.

142 The required test temperature is 12°C, which corresponds to the average environmental temperature for the EU (Guidance on IRs and CSA, Table R.16-8) and is in line with the applicable test conditions of the OECD TG 308.

143 In accordance with the specifications of the OECD TG 308, non-extractable residues (NER) must be quantified. The reporting of results must include a scientific justification of the used

extraction procedures and solvents (Guidance on IRs and CSA, Section R.7.9.4.1.). 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) (Guidance on IRs and CSA, Section R.11.4.1.1.3.). Further recommendations may be found in the background note on options to address non-extractable residues in regulatory persistence assessment available on the ECHA website.

144 Relevant transformation/degradation products are at least those detected at ≥ 10% of the applied dose at any sampling time or those that are continuously increasing during the study even if their concentrations do not exceed 10% of the applied dose, as this may indicate persistence (OECD TG 308; Guidance on IRs and CSA, Section R.11.4.1.).

9. Identification of degradation products

145 Further degradation testing must be considered if the chemical safety assessment (CSA) according to Annex I indicates the need to investigate further the degradation of the substance (Annex VIII, Section 9.2., Column 2).

146 This information requirement is triggered in case the chemical safety assessment (CSA) indicates the need for further degradation investigation (Annex I, Section 4; Annex XIII, Section 2.1), such as if the substance is a potential PBT/vPvB substance (Guidance on IRs and CSA, Section R.11.4.).

147 As already explained in Section 6, the Substance is a potential PBT/vPvB substance.

148 Therefore, the chemical safety assessment (CSA) indicates the need for further degradation investigation.

149 In your comments on the draft decision, you agree to identify degradation products in one of the simulation studies.

9.1. *Study design and test specifications*

150 Identity, stability, behaviour, and molar quantity of the degradation/transformation products relative to the Substance must be evaluated and reported, when analytically possible. In addition, degradation half-life, log K_{ow} and potential toxicity of the transformation/degradation may need to be investigated. You must obtain this information from one of the degradation studies requested in the Requests in Sections 6-8..

151 To determine the degradation rate of the Substance, the requested study according to the OECD TG 309 (Request in Section 6) must be conducted at 12°C and at a test concentration < 100 µg/L. However, to overcome potential analytical limitations with the identification and quantification of major transformation/degradation products, you may consider running a parallel test at higher temperature (but within the frame provided by the test guideline, e.g. 20°C) and at higher application rate (i.e. > 100 µg/L).

152 To determine the degradation rate of the Substance, the requested studies according to the OECD TGs 308/307 (Requests in Sections 7 or 8) must be conducted at 12°C and at test material application rates reflecting realistic assumptions. However, to overcome potential analytical limitations with the identification and quantification of major transformation/degradation products, you may consider running a parallel test at higher temperature (but within the frame provided by the test guideline) and at higher application rate (e.g. 10 times).

References

The following documents may have been cited in the decision.

Guidance on information requirements and chemical safety assessment (Guidance on IRs & CSA)

Chapter R.4 Evaluation of available information; ECHA (2011).
Chapter R.6 QSARs, read-across and grouping; ECHA (2008).
Appendix to Chapter R.6 for nanoforms; ECHA (2019).
Chapter R.7a Endpoint specific guidance, Sections R.7.1 – R.7.7; ECHA (2017).
Appendix to Chapter R.7a for nanomaterials; ECHA (2017).
Chapter R.7b Endpoint specific guidance, Sections R.7.8 – R.7.9; ECHA (2017).
Appendix to Chapter R.7b for nanomaterials; ECHA (2017).
Chapter R.7c Endpoint specific guidance, Sections R.7.10 – R.7.13; (ECHA 2017).
Appendix to Chapter R.7a for nanomaterials; ECHA (2017).
Appendix R.7.13-2 Environmental risk assessment for metals and metal compounds; ECHA (2008).
Chapter R.11 PBT/vPvB assessment; ECHA (2017).
Chapter R.16 Environmental exposure assessment; ECHA (2016).

Guidance on data-sharing; ECHA (2017).

All Guidance on REACH is available online: https://echa.europa.eu/guidance-documents/guidance-on-reach

Read-across assessment framework (RAAF)

RAAF, 2017 Read-across assessment framework (RAAF), ECHA (2017)
RAAF UVCB, 2017 Read-across assessment framework (RAAF) – considerations on multi- constituent substances and UVCBs), ECHA (2017).

The RAAF and related documents are available online:
https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across

***OECD Guidance documents* (OECD GDs)**

OECD GD 23 Guidance document on aquatic toxicity testing of difficult substances and mixtures; No. 23 in the OECD series on testing and assessment, OECD (2019).
OECD GD 29 Guidance document on transformation/dissolution of metals and metal compounds in aqueous media; No. 29 in the OECD series on testing and assessment, OECD (2002).
OECD GD 150 Revised guidance document 150 on standardised test guidelines for evaluating chemicals for endocrine disruption; No. 150 in the OECD series on testing and assessment, OECD (2018).
OECD GD 151 Guidance document supporting OECD test guideline 443 on the extended one-generation reproductive toxicity test; No. 151 in the OECD series on testing and assessment, OECD (2013).

Appendix 2: Procedure

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

ECHA followed the procedure detailed in Articles 50 and 51 of REACH.

The compliance check was initiated on 16 June 2021.

ECHA notified you of the draft decision and invited you to provide comments. ECHA took into account your comments and modified request 4.

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

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

The deadline of the decision is set based on standard practice for carrying out OECD TG tests. It has been exceptionally extended by 12 months from the standard deadline granted by ECHA to take into account currently longer lead times in contract research organisations.

Appendix 3: Addressees of this decision and their corresponding information requirements

In accordance with Articles 10(a) and 12(1) of REACH, the information requirements for individual registrations are defined as follows:

- the information specified in Annex VII to REACH, for registration at 1-10 tonnes per year (tpa), or as a transported isolated intermediate in quantity above 1000 tpa;
- the information specified in Annexes VII and VIII to REACH, for registration at 10-100 tpa;
- the information specified in Annexes VII, VIII and IX to REACH, for registration at 100-1000 tpa;
- the information specified in Annexes VII to X to REACH, for registration at more than 1000 tpa.

Registrant Name	Registration number	Highest REACH Annex applicable to you
[redacted]	[redacted]	[redacted]
[redacted]	[redacted]	[redacted]

Where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas ECHA will send the decision to the actual registrant.

Appendix 4: Conducting and reporting new tests for REACH purposes

1. Requirements when conducting and reporting new tests for REACH purposes

1.1. Test methods, GLP requirements and reporting

(1) 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.

(2) 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.

(3) 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[2].

1.2. Test material

153 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 must be selected taking into account 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. For example, if a constituent/ impurity of the Substance is known to have an impact on (eco)toxicity, the selected Test Material must contain that constituent/ impurity.

(2) Information on the Test Material needed in the updated dossier

- 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.
- The reported composition must include all constituents of each Test Material and their concentration values and other parameters relevant for the property to be tested.

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 on How to prepare registration and PPORD dossiers[3].

[2] https://echa.europa.eu/practical-guides
[3] https://echa.europa.eu/manuals

2. General recommendations for conducting and reporting new tests

2.1. Strategy for the PBT/vPvB assessment

Under Annex XIII, the information must be based on data obtained under conditions relevant for the PBT/vPvB assessment. You must assess the PBT properties of each relevant constituent of the Substance present in concentrations at or above 0.1% (w/w) and of all relevant transformation/degradation products. Alternatively, you would have to justify why you consider these not relevant for the PBT/vPvB assessment.

You are advised to consult Guidance on IRs & CSA, Sections R.7.9, R.7.10 and R.11 on PBT assessment to determine the sequence of the tests needed to reach the conclusion on PBT/vPvB. The guidance provides advice on 1) integrated testing strategies (ITS) for the P, B and T assessments and 2) the interpretation of results in concluding whether the Substance fulfils the PBT/vPvB criteria of Annex XIII.

In particular, you are advised to first conclude whether the Substance fulfils the Annex XIII criteria for P and vP, and then continue with the assessment for bioaccumulation. When determining the sequence of simulation degradation testing you are advised to consider the intrinsic properties of the Substance, its identified uses and release patterns as these could significantly influence the environmental fate of the Substance. You must revise your PBT assessment when the new information is available.

Depending on the potential persistence (P/vP criteria met) of the Substance and/or its relevant degradation/hydrolysis products and the experimentally derived logKow value, as requested in this decision, you are advised to consider the need to submit a testing proposal to further investigate the bioaccumulation of the Substance or its relevant degradation/hydrolysis product(s) for the PBT/vPvB assessment.