Helsinki, 28 November 2016

Addressee
[redacted]

Decision number: CCH-D-2114348828-34-01/F
Substance name: bis(dibutyldithiocarbamato-S,S')copper
EC number: 237-695-7
CAS number: 13927-71-4
Registration number: [redacted]
Submission number: [redacted]
Submission date: 21.08.2013
Registered tonnage band: 100-1000 tonnes per year

DECISION ON A COMPLIANCE CHECK

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

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

2. **Granulometry (Annex VII, Section 7.14.; test method: using an appropriate test method) with the registered substance;**

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

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

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

6. **Identification of degradation products (Annex IX, 9.2.3.) using an appropriate test method with the registered substance;**

7. **Bioaccumulation in aquatic species (Annex IX, Section 9.3.2.; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD TG 305, dietary exposure) with the registered substance;**

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

You are required to submit the requested information in an updated registration dossier by **4 June 2019**. You shall also update the chemical safety report, where relevant.

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

Appeal

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

Authorised[1] by Ofelia Bercaru, Head of Unit, Evaluation E3

[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.

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Appendix 1: Reasons

IDENTIFICATION OF THE SUBSTANCE

In order to ensure that potential hazardous properties of the substance are not underestimated, the information that is necessary to resolve the substance identification deficiencies below, must be available to you before identifying the test sample to be used for the testing requested in the present decision.

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

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

Annex VI, section 2.3.7 of the REACH Regulation requires that each registration dossier contains a sufficiently detailed description of the analytical method used for establishing the composition of the registered substance and therefore its identity. This information shall be sufficient to allow the method to be reproduced.

Your substance is identified as bis(dibutyldithiocarbamato-S,S')copper, however it is missing the description of the analytical methods used to:

i) Identify and quantify the copper counter-ion;

ii) Determine the ratio between the organic ligand dibutyldithiocarbamato-S,S' and the copper ion;

Therefore, your dossier does not have sufficient information to verify the reported composition of the registered substance and therefore its identity.

Accordingly, you are required to provide the description of the analytical method used on the identification and quantification of the counter-ion and on the analytical method used to determine the ratio between the organic ligand dibutyldithiocarbamato-S,S' and the copper ion (e.g elemental analysis).

The description shall be sufficient for the methods to be reproduced and shall therefore include details of the experimental protocol followed, any calculation made and the results obtained.

You shall ensure that the analytical data provided on the quantification of the substance is consistent with the composition and identity reported for the substance.

As for the reporting of the data in the registration dossier, the information should be attached in IUCLID section 1.4.

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PROPERTIES OF THE SUBSTANCE

Grouping of substances and read-across approach

Article 13(1) of the REACH Regulation provides that information on intrinsic properties of substances may be generated by means other than tests. Such other means include the use of information from structurally related substances (grouping of substances and read-across), "provided that the conditions set out in Annex XI are met".

In the registration, you have adapted the standard information requirements for

- Repeated Dose Toxicity sub-chronic study (90-day) (Annex IX, Section 8.6.2.)
- Pre-natal Developmental Toxicity study (Annex IX, Section 8.7.2.)

by applying a read-across adaptation following REACH Annex XI, Section 1.5.

Annex XI, Section 1.5., requires a structural similarity among the substances within a group or category such that relevant properties of a substance within the group can be predicted from the data on reference substance(s) within the group by interpolation. The following analysis presents your justification for the proposed grouping approach and read-across hypothesis, together with ECHA's analysis concerning the justification in both a generic and a property-specific context.

A. Description of the grouping and read-across approach proposed by the Registrant

You have provided a read-across justification as a separate attachment under Assessment Reports (section 13 of IUCLID) in the registration. In summary you provide the following arguments to support the read-across approach:

Hypothesis for the analogue approach:

"The analogue approach is based on read-across to substances with the same chemical structures (dithiocarbamate), similar physicochemical properties and toxicological profiles. Dithiocarbamate substances could be suitable as source chemicals to fill by read-across the registration dossier of the target substance: Copper dibutyldithiocarbamate (CAS N. 13927-71-4). For the toxicological part, this read-across approach is based on the hypothesis that the toxicity of copper dibutyldithiocarbamate is due to the dithiocarbamate function and not due to copper. The analogue approach is proposed to fulfil the CDBC data gap for the acute toxicity by dermal route, the repeated toxicity and the developmental toxicity endpoints."

"Copper dibutyldithiocarbamate (CDBC) has a high structural similarity with zinc dibutyldithiocarbamate (ZDBC) and zinc diethyldithiocarbamate (ZDEC). CDBC and ZDBC are two dibutylthiocarbamates but they have a different cation: copper/zinc. CDBC and ZDEC differ in the length of the aliphatic chain: CDBC contains four butyls (4 carbons) and ZDEC, four ethyls (2 carbons)."

ECHA considers this as the hypothesis under which you make predictions for the properties listed above.

B. ECHA analysis of the grouping and read-across approach in light of the requirements of Annex XI, 1.5.

With regards to the proposed predictions ECHA has the following observations:

Explanation on why and how the structural similarities allow predictions

In order to meet the provisions in Annex XI, Section 1.5., to predict human health effects from data for a reference substance within the group by interpolation to other substances in the group, ECHA considers that structural similarity alone is not sufficient. It has to be justified why such prediction is possible in view of the identified structural differences and the provided evidence has to support such explanation. In particular, the structural similarities must be linked to a scientific explanation of how and why a prediction is possible.

The justification states that "*the analogue approach is based on read-across to substances with the same chemical structures (dithiocarbamate), similar physicochemical properties and toxicological profiles*".

ECHA notes the following:

a. Structural similarity is a prerequisite for applying the grouping and read-across approach, but ECHA does not accept in general or this specific case that structural similarity per se is sufficient to enable the prediction of human health properties of a substance, since structural similarity does not always lead to predictable or similar human health properties. Hence, further elements are needed such as a well-founded hypothesis of (bio)transformation to a common compound(s), or that different compounds have the same type of effect(s), to allow a prediction of human health properties that does not underestimate risks.

b. Similar physical and chemical properties is a prerequisite for applying the grouping and read-across approach, but ECHA does not accept in general or this specific case that similar physical and chemical properties per se is sufficient to enable the prediction of human health properties of a substance, since similar physical and chemical properties does not always lead to predictable or similar human health properties. Hence, further elements are needed to allow a prediction of human health properties that does not underestimate risks.

c. ECHA considers that "*similar toxicological profiles*" are not in themselves a robust basis for predicting the properties of a substance, since there are many substances which share a number of toxicological properties, but then differ in other toxicological properties. ECHA also notes that in this case, the amount of information for the target substance which is in common and is comparable to the source substances is limited. The only test that obtained comparable results among the three substances is the *in vitro* gene mutation test. The tests on skin irritation, eye irritation and skin sensitisation show comparable results only between the two source substances and not with the target substance.

Moreover, there are some differences in the toxicological profile, which have not been accounted for. Both source substances, ZDBC and ZDEC, are classified as skin irritant cat. 2, eye irritant cat 2, STOT SE 3, and ZDEC is classified as Acute Tox. 4; however the target substance is not classified as such. ZDEC resulted positive to the *in vitro* cytogenicity study whilst CDBC achieved a negative result. The NOAEL for CDBC obtained from the sub-acute (oral) repeated dose toxicity is 1000mg/kg while the NOAEL levels for ZDBC and ZDEC, from sub-chronic (oral) repeated dose toxicity, are 41 and <36mg/kg, respectively. The data provided shows that the source substances chosen for read-across have significant differences with the target substance. These differences contradict your hypothesis that these substances have a similar toxicological profile. This further undermines the use of similar toxicological profile as a basis for predicting the properties of the registered substance.

You also proposed that ZDEC is more toxic than the registered substance, and hence can be used as a worst case. However, as set out above, ECHA considers that there is no reliable basis whereby ZDEC can be predicted to be a worst case for the toxicological properties of the registered substance. ECHA considers that the requirement of Annex XI, 1.5., that human health effects may be predicted from data for reference substance(s) within the group by interpolation to other substances in the group (read-across approach), has not been met.

d. You compared three substances with a dithiocarbamate function, which have additionally other structural differences, and have thus derived the hypothesis that "*the toxicity of copper dibutyldithiocarbamate is due to the dithiocarbamate function*". However, ECHA considers that it is not legitimate to conclude that the dithiocarbamate function is responsible for toxicity on this factual basis, since the comparison does not adequately take into account the possible contribution of other functional differences in the substances. ECHA therefore considers that, on this basis, the hypothesis is not sufficient to make a reliable prediction of the properties of the registered substance.

   According to the data matrix provided, the two source substances achieved a negative and a positive result for the *in vitro* cytogenicity test. Moreover, only ZDEC is classified as acute toxicity 4. These observations show that though the source substances have the same dithiocarbamate structure they have different toxicological properties, hence the toxicity does not totally depend on this "*dithiocarbamate function*". On this basis, ECHA also considers that your hypothesis, that the dithiocarbamate function controls toxicity, is not a reliable basis for prediction and the requirement of Annex XI, 1.5., that human health effects may be predicted from data for reference substance(s) within the group by interpolation to other substances in the group (read-across approach), has not been met.

ECHA concludes that you have not addressed the obvious structural differences between the source substances and the target substance and did not explain why those differences would not lead to differences in the toxicity profile of target and source substances. The provided explanation is not considered as valid to establish a scientifically credible link between the structural similarity and the prediction.

C. Conclusion on the read-across approach

On the basis of the analysis carried out above, ECHA concludes, that you have failed to meet the requirement of Annex XI, Section 1.5., that human health effects may be predicted from data for reference substance(s) within the group by interpolation to other substances in the group (read-across approach).

The adaptation of the standard information requirements for the endpoints of repeated dose toxicity and reproductive toxicity in the technical dossier is based on the proposed read-across approach examined above. ECHA does not consider your read-across justification to be a reliable basis to predict the properties of the registered substance for the reasons set out above. Thus, the provided adaptation does not comply with the general rules of adaptation as set out in Annex XI, 1.5. Therefore, ECHA rejects all adaptations in the technical dossier that are based on Annex XI, 1.5.

2. Granulometry (Annex VII, Section 7.14.)

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(d) of the REACH Regulation, your technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation.

"Granulometry" is a standard information requirement as laid down in Annex VII, Section 7.14 of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

In the technical dossier you have provided a study record for a [redacted] (2009)/K1 KS/Particle size distribution (sieving). Based on the provided study using OECD TG 110 (Particle size distribution/Fibre length and diameter distribution) sieving, you reported the following: *"According to a granulometry study (sieving) OECD 110, 42.3% of the particles have a size > 500 µm and so 57.7% have a size < 500 µm.* However, this study does not provide the information required by Annex VII, Section 7.14., because the reported study only distinguishes between particles larger and smaller than 500 µm = 0.5 mm. According to OECD TG 110, the quality criteria for both methods A and B demand that much smaller particles than 500 µm "*must be measureable*" (OECD TG 110 at 2.A under "Quality criteria", "Sensitivity" on page 7). Furthermore, ECHA notes that the provided level of test sensitivity and reporting detail is not adequate for risk assessment, due to remaining uncertainty of the transportation and sedimentation behaviour of the particles.

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

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Granulometry using an appropriate test method.

ECHA acknowledges that in your comments you have expressed your intention to provide additional information on granulometry through a dossier update. Any new information will be assessed at the follow-up stage.

Guidance for determining appropriate test methods for the granulometry endpoint is available in the ECHA Guidance on information requirements and chemical safety assessment R.7a, chapter R.7.1.14.3 (July 2015).

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

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(d) and 13(4) of the REACH Regulation, your technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation.

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

You have proposed to adapt this information requirement according to Annex XI, Section 1.5. of the REACH Regulation by providing a study record for a 17-week sub-chronic study (no guideline followed and non-GLP compliant) with the analogue substance Zinc dibutyldithiocarbamate (ZDBC) (EC no 205-232-8). However, as explained above in this Appendix 1, the adaptation of the information requirement cannot be accepted.

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

ECHA has evaluated the most appropriate route of administration for the study. Based on the information provided in the technical dossier and/or in the chemical safety report, ECHA considers that the oral route - which is the preferred one as indicated in ECHA *Guidance on information requirements and chemical safety assessment* (version 4.1, October 2015) Chapter R.7a, section R.7.5.4.3 - is the most appropriate route of administration. More specifically, even though the information indicates that human exposure to the registered substance by the inhalation route is likely, the test substance has a very low vapour pressure ($6.4x10^{-12}$Pa at 25°C), a high boiling point of (>300°C), is not classified as skin/eye irritant and there are no professional or consumer uses for this substance. It seems that there is no concern for inhalation exposure. Hence, the test shall be performed by the oral route using the test method EU B.26./OECD TG 408.

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

In your comments to the draft decision you agreed to perform a sub-chronic toxicity study (90 day) by oral route in rats according to the TG OECD 408.

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

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

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(d) and 13(4) of the REACH Regulation, your technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation.

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

You have proposed to adapt this information requirement according to Annex XI, Section 1.5., of the REACH Regulation by providing a study record for the prenatal and postnatal developments of rats (no guideline followed/non-GLP compliant), with the analogue substance Zinc diethyldithiocarbamate (EC no 238-270-9). However, as explained above in this Appendix 1, the adaptation of the information requirement cannot be accepted.

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

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

ECHA considers that the oral route is the most appropriate route of administration for substances except gases to focus on the detection of hazardous properties on reproduction as indicated in ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, July 2015) R.7a, chapter R.7.6.2.3.2. Since the substance to be tested is a solid, ECHA concludes that testing should be performed by the oral route.

In your comments to the draft decision you agreed to to perform a pre-natal developmental toxicity study by oral route in rats according to the TG OECD 414.

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

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

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(d) and 13(4) of the REACH Regulation, a technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation.

"Sediment simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.4. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex IX, Section 9.2., column 2. You provided the following justification for the adaptation*: "Further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The choice of the appropriate test(s) depends on the results of the chemical safety assessment and may include simulation testing in appropriate media (e.g. water, sediment or soil). As the chemical safety assessment is not yet performed due to lack of toxicity up to the water solubility limit (EPM not realisable), no simulation test is proposed".*

ECHA notes that the provided adaptation needs to meet the criteria of either the specific adaptation rules of Column 2 of Annex IX, Section 9.2 or the general adaptation rules of Annex XI in order to fulfil the standard information requirements.

ECHA further notes that your adaptation does not meet the specific rules for adaptation of Annex IX, Section 9.2.1.4., column 2 because you have not provided any justification in the technical dossier or the chemical safety assessment for why there is no need to investigate further the degradation on the substance and its degradation products and the provided adaptation refers to missing information, namely exposure and risk assessment.

Furthermore, according to Annex IX, Section 9.2.1.4, column 2 of the REACH Regulation, sediment simulation testing does not need to be conducted if the substance is readily biodegradable or if direct and indirect exposure of sediment is unlikely. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable in OECD 301F test (0%), has low water solubility (1 µg/L), high partition coefficient (log Kow 4.7) and high adsorption coefficient (log Koc 5.6), indicating adsorptive properties. Furthermore, ECHA considers that sediment exposure cannot be excluded as there are no exposure estimations in the Chemical Safety Report (CSR). ECHA therefore considers that you have not in your CSR demonstrated that indirect and direct sediment exposure is unlikely.

Therefore, the registered substance cannot be considered readily biodegradable and indirect and direct exposure to sediment cannot be excluded and need to investigate further the degradation based on the chemical safety assessment cannot be excluded. Consequently, you have not demonstrated that the specific rules for adaptation presented in column 2 of Annex IX, Section 9.2.1.4 of the REACH Regulation are met.

Column 1 of Annex IX establishes the standard information requirements for substances registered from 100 to 1000 tonnes per annum. The specific rules for adaptation in column 2 of the Annex provide exceptions to this (see introductory paragraph 2 to Annex IX). Accordingly, degradation testing in Annex IX, 9.2.1. may be omitted based on the results of the chemical safety assessment. In your adaptation you refer to the chemical safety assessment not being performed yet due to lack of toxicity up the water solubility limit. Thus, you have not provided an appropriate documentation to show that the CSR would indicate that there is no need for simulation testing.

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

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

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 2.0, November 2014) Aerobic and anaerobic transformation in aquatic sediment systems (test method EU C.24. / OECD TG 308) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.4.

One of the purposes of the simulation test is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of REACH Regulation to decide whether it is persistent in the environment. Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 2.0, November 2014) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment".

The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation, Table R.16-9 (version 2.1 October 2012) indicates 12°C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment. Performing the test at the temperature of 12°C is within the applicable test conditions of the Test Guideline OECD TG 308. Therefore, the test results, and in particular the degradation rates, should correspond to the temperature of 12°C.

ECHA acknowledges your comments on the request for sediment simulation test and identification of the degradation products (section 6). In your comments you argue that carrying out degradation simulation testing and degradation products identification is not required at this stage in any compartment.

In line with your comments, ECHA agrees that "Aerobic and anaerobic" in the context of sediment simulation test 308 OECD refers to the name of the test guideline only. The test shall be performed according to the standard OECD 308 TG following the guidance for testing the degradation in aerobic sediment system. The testing in strictly anaerobic sediment system is not required.

In your comments you also refer to a series of ongoing ecotoxicity testing (long-term aquatic toxicity, toxicity to sediment organisms and long-term terrestrial toxicity) under Article 40 of the REACH Regulation (ECHA decision 26 January 2015) and your intention to update the Chemical Safety Assessment (CSA) after the information on these studies is available. In your comments you further refer to the waiver on the simulation tests in relation to the evaluation of the testing proposals. According to you, as the CSA was not yet performed due to lack of toxicity up to the water solubility limit (EPM not realisable), no simulation tests were proposed.

ECHA points out that under the above testing proposal evaluation on ecotoxicity endpoints, ECHA did not evaluate any adaptation on the degradation endpoints since there was no testing proposal for degradation

You have information on the biodegradation of the substance demonstrating no degradation of the substance in the screening level assessment. Based on the available screening level information on biodegradation, it is not possible to conclude on persistency and there is no information on potential degradation products. Therefore, ECHA notes that the PBT/vPvB properties of the substance and its degradation products needs to be assessed regardless on the outcome of the ongoing ecotoxicity tests.

ECHA further notes that a PBT/vPvB assessment is required for all substances for which a CSA must be conducted. CSA needs to be provided for all substance manufactured or imported in quantities of 10 tonnes per year and more (Article 14(1) of the REACH Regulation).

You may seek waiving testing if the adaptation meets either the specific adaptation rules of column 2 of Annex IX, Section 9.2 of the REACH Regulation or general rules for adaptation set in Annex XI. However, lack of information does not fulfil the criteria for successful adaptation.

In your comments on the Bioaccumulation testing you state that no biodegradation was observed within 28 days in the ready biodegradability test (OECD 301F guideline) and no microorganism inhibition took place. In addition, you expect no significant biodegradation under simulation degradation testing at 12°C resulting in conclusions that the registered substance would be at least P. Therefore, you propose to first conduct the B/vB investigation.

As there is no information on potential degradation products and no degradation was observed during screening assessment, ECHA agrees that testing at 12°C might not be beneficial in identification of the degradation products. Therefore ECHA concludes that the request for the testing at the specific temperature (12°C) can be removed and you may perform the simulation test in the temperature range described in the OECD TG. As stated above, the results, and in particular the degradation rates, should however correspond to the temperature of 12°C. ECHA notes that according to the Guidance on information requirements and chemical safety assessment R.7b (version 3.0, February 2016) temperature correction of degradation half-lives from available study results to 12°C is recommended and should be based on the Arrhenius equation.

The time line of this decision allows the sequential testing of the persistence and bioaccumulation. However, according to ECHA Guidance R11 (November 2014) standard approach in the PBT/vPvB assessment must cover the substance, its constituents, impurities, additives or transformation/degradation products. When for several properties further information is needed, the persistence assessment should be conducted in parallel with the screening level assessment for bioaccumulation or before bioaccumulation testing. In this case even if the substance, according to you, is likely to be P, there is no information on potential degradation products. This is important to be clarified before starting the bioaccumulation assessment to avoid unnecessary vertebrate testing.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic and anaerobic transformation in aquatic sediment systems (test method: EU C.24./OECD TG 308).

Notes for your consideration

In accordance with Annex I, Section 4, of the REACH Regulation you should revise the PBT assessment when results of the test detailed above is available. You are also advised to consult the ECHA Guidance on information requirements and chemical safety assessment (version 2.0, November 2014), Chapter R.11, Section R.11.4.1.1. and Figure R. 11-3 on PBT assessment for the integrated testing strategy for persistency assessment in particular taking into account the degradation products of the registered substance.

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

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(d) and 13(4) of the REACH Regulation, your technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation.

The identification of the degradation products is a standard information requirement according to column 1, Section 9.2.3. of Annex IX of the REACH Regulation. Column 2 of Section 9.2.3. of Annex IX further states that the information does not need to be provided if the substance is readily biodegradable.

ECHA notes that, as described above in the section (5) the registered substance is not readily biodegradable and you have intended to cover the adaptation of the information requirement for the identification of the degradation products with the following justification; "Further biotic degradation testing shall be proposed by the registrant if the chemical safety assessment according to Annex I indicates the need to investigate further the degradation of the substance and its degradation products. The choice of the appropriate test(s) depends on the results of the chemical safety assessment and may include simulation testing in appropriate media (e.g. water, sediment or soil)." As explained in the section 5 of this decision your adaptation does not meet the specific rules for adaptation of Annex IX, Section 9.2.1.4., column 2 because you have not provided any justification in the technical dossier for why there is no need to identify the degradation products and the provided adaptation refers to missing information, namely exposure and risk assessment.

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

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

Therefore, pursuant to Article 41(1)(a) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision:

Identification of the degradation products using an appropriate and suitable test method, as explained above in this section.

Notes for your consideration

Before providing the above information you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment* (version 2.0, November 2014), Chapter R.7b., Sections R.7.9.2.3 and R.7.9.4.

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

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(d) and 13(4) of the REACH Regulation, your technical dossier registered at 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes VII to IX of the REACH Regulation.

"Bioaccumulation in aquatic species, preferably fish" is a standard information requirement as laid down in Annex IX, Section 9.3.2. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement. While you have not explicitly claimed an adaptation, you have provided information that could be interpreted as an attempt to adapt the information requirement according to Annex XI, Section 1.3. You provided the following information to support the adaptation: Results from a quantitative structure-activity relationship model ((Q)SAR), BCFBAF model v3.01 from EPI Suite v4.1 resulting in an estimated bioconcentration factor (BCF) of "*Log BCF = 1.414 (BCF = 25.92 L/kg wet-wt)*".

In the technical dossier you state that "*BCFBAF model v3.01 from EPI Suite v4.1, which fulfilled all OECD principles. Test substance is within the domain of the BCFBAF model based on the molecular weight and fragments present in the BCFBAF database*".
Article 13(1) of the REACH Regulation stipulates that information on intrinsic properties of substances may be generated by means other than tests, provided that the conditions set out in Annex XI are met. According to Section 1.3 of the Annex XI, results obtained from valid qualitative or quantitative structure-activity relationship models ((Q)SARs) may indicate the presence or absence of a certain dangerous property. Results of (Q)SARs may be used instead of testing when the following conditions are met:

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

Regarding the applicability domain of the model, you state that the "*estimation domain for BCF is based on the number of instances given for each correction factor in any of the training set compounds, and the minimum and maximum values for molecular weight and log Kow.*" In the description of the algorithm you further elaborate that "*BCFBAF v3.01 contains two methods for estimating BCFs. The first BCFBAF method is based on the original BCFWIN model and classifies a compound as either ionic or non-ionic. Ionic compounds include carboxylic acids, sulfonic acids and salts of sulfonic acids, and charged nitrogen compounds (nitrogen with a +5 valence such as quaternary ammonium compounds). All other compounds are classified as non-ionic.*"

ECHA notes that you have not provided sufficient evidence to support the assumption that the substance would fall within the applicability domain of the model. You refer to "*Estimation Domain*" showing the applicability domain with regards to molecular weight and logKow. However, the source publication Meylan et al. 1999 describes that "*Organometallics, nonionics with long alkyl chains, and aromatic azo compounds receive special treatment*". In your registration dossier you state that the correction "*Alkyl chains (8+ -CH2- groups): -1.374*" was used in the equation to estimate the BCF (i.e., "*Log BCF = 0.6598 log Kow - 0.333 + Correction*"). ECHA notes that this correction does not consider copper (Cu) present in the registered substance. In fact, none of the substances in the training set contains copper and therefore it is unlikely that the model could predict property of the registered substance.

ECHA notes that your adaptation does not meet the general rule for adaptation of Annex XI; Section 1.3., because, taking into consideration the above mentioned deficiencies, ECHA considers that the substance does not fall within the applicability domain of the model. Therefore, your adaptation of the information requirement cannot be accepted.

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

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7c* (version 2.0, November 2014) bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to cover the standard information requirement of Annex IX, Section 9.3.2. Since the low water solubility of the registered substance (1 µg/L) among the high adsorption potential (log Kow 4.7 and log Koc 5.6) may lead to technical problems in conducting OECD 305 with aquatic exposure, dietary exposure is requested.
In your comments to the draft decision you agree that there is a need for further information on persistency and bioaccumulation. You assume that the registered substance is at least persistent. Therefore you propose a testing strategy to perform first the bioaccumulation test prior to simulation test in sediment.

For the PBT-assessment, the ECHA Guidance R.11 (November 2014) Figure R.11-4 states that, generally the B- assessment starts only if substance fulfils the P or vP criteria. As stated above under section 5 the standard approach is to perform first the P assessment followed by B assessment. According to the ECHA Guidance R.11 (November 2014) standard approach in the PBT/vPvB assessment must cover the substance, its constituents, impurities, additives or transformation/degradation products. When for several properties further information is needed, the persistence assessment should be conducted in parallel with the screening level assessment for bioaccumulation or before bioaccumulation testing. In this case even if the substance, according to you, is likely to be P, there is no information on potential degradation products. This is important to be clarified before starting the bioaccumulation assessment to avoid unnecessary vertebrate testing.

In your comments you have no objection for performing an OECD 305 test with dietary exposure. Reason for this is the knowledge you have gained on CDBC behaviour in water when carrying out still undergoing long-term aquatic toxicity studies. During the testing you have concluded that it would be technically impossible to keep steady concentrations of CDBC in water, even under flow-through systems due to very low solubility, analytical difficulties etc. The concern you raised in your comments was the acceptability of the results from the dietary study in relation to the cut-off criteria set out under REACH Annex XIII for B/vB assessment being based on BCF values only. You believe that a set of BCFs derived from different sets of relevant equations (Crookes and Brooke, 2011) applicable to the registered substance, dietary test (BMF) would be sufficient to build a WoE to decide on the B/vB properties.

ECHA acknowledges your concern regarding the acceptability of the dietary study results in PBT/vPvB assessment. ECHA notes that the OECD 305 gives preference for aquatic exposure whenever possible. Therefore it is important that you transparently justify the selected exposure route. Based on your comments, ECHA understands that you have explored all means to create stable test item concentrations in water and has concluded that such testing is technically not feasible.

ECHA notes that OECD TG 305-III (dietary exposure) includes details on what parameters to report and how to calculate the BCF based on results on dietary exposure. These are in line with your comments. The OECD TG 305 lists the parameters to be reported for dietary study. In addition, Annex 8 of the OECD TG 305 includes information on the estimation of the tentative BCFs from data collected in the dietary exposure study. By applying these available techniques to estimate k1 (and so BCF), estimation of the bioaccumulation potential could be achieved. Based on the above ECHA concludes that comparison of the results with the BCF criteria set in Annex XIII should be possible. Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision Bioaccumulation in fish: dietary exposure bioaccumulation fish test (test method: OECD TG 305-III).

Notes for your consideration

Before conducting the above test you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment* (version 2.0, November 2014), Chapter R.11.4. and Figure R.11-4 on the PBT assessment for further information on the integrated testing strategy for the bioaccumulation assessment of the registered substance. You should revise the PBT assessment when information on bioaccumulation is available.

Deadline to submit the requested information in this decision

In the draft decision communicated to you the time indicated to provide the requested information was 24 months from the date of adoption of the decision. In your comments on the draft decision, you requested an extension of the timeline to 36 months. You sought to justify this request by time needed to complete the bioaccumulation study. You demonstrated the challenges in the development of the validated analytical tools, radiolabelling of the substance and uncertainty of the availability of the facilities of the service provider.

ECHA evaluated the justification provided. You have provided justification letter with the information that validated analytical method for CDBC in water could be expected in April 2016 at best if the new intended analytical method works out. In addition you have described the analytical difficulties with the registered substance. You have not included documentation on the potential lack of facilities in performing the bioaccumulation study.

Therefore, ECHA has only partially granted the request and set the deadline to 30 months.

Appendix 2: Procedural history

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

The compliance check was initiated on 11 December 2015.

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

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

ECHA took into account your comments and amended the request(s) and the deadline.

ECHA notified the draft decision to the competent authorities of the Member States for proposal(s) for amendment.
ECHA received proposal(s) for amendment and modified the draft decision.

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

ECHA referred the draft decision to the Member State Committee.
Your comments on the proposed amendment(s) were taken into account by the Member State Committee.

In addition, you provided comments on the draft decision. These comments were not taken into account by the Member State Committee as they were considered to be outside of the scope of Article 51(5).

The Member State Committee reached a unanimous agreement on the draft decision in its MSC-50 written procedure and ECHA took the decision according to Article 51(6) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

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

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

3. In carrying out the test(s) required by the present decision it is important to ensure that the particular sample of substance tested is appropriate to assess the properties of the registered substance, taking into account any variation in the composition of the technical grade of the substance as actually manufactured or imported. If the registration of the substance covers different grades, the sample used for the new test(s) must be suitable to assess these. Furthermore, there must be adequate information on substance identity for the sample tested and the grade(s) registered to enable the relevance of the test(s) to be assessed.