ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 1 August 2017

Addressee: [redacted]

Decision number: CCH-D-2114366654-41-01/F
Substance name: Bis(2,6-diisopropylphenyl)carbodiimide
EC number: 218-487-5
CAS number: 2162-74-5
Registration number: [redacted]
Submission number: [redacted]
Submission date: 10.02.2017
Registered tonnage band: 100-1000T

DECISION ON A COMPLIANCE CHECK

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

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

2. Sediment simulation testing (Annex IX, Section 9.2.1.4.; test method: Aerobic and anaerobic transformation in aquatic sediment systems, EU C.24./OECD TG 308) at a temperature of 12 °C with the registered substance;

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

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

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

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

You may adapt the testing requested above according to the specific rules outlined in Annexes VI to IX and/or according to the general rules contained in Annex XI to the REACH Regulation. 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 adequate and reliable documentation.

You have to submit the requested information in an updated registration dossier by **10 February 2020**. You also have to update the chemical safety report, where relevant. The timeline has been set to allow for sequential testing.

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

Appeal

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

Authorised[1] by Claudio Carlon, Head of Unit, Evaluation E2

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

Appendix 1: Reasons

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

"Soil simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.3. of the REACH Regulation for substances with a high potential for adsorption to soil. The registered substance has low water solubility (<0.05 mg/L), high partition coefficient (log Kow >6.2) and high adsorption coefficient (log Koc,soil >5), indicating high adsorptive properties. Therefore, adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have sought to adapt this information requirement according to Annex IX, Section 9.2.1.3., column 2. You provided the following justification for the adaptation: *"No exposure to soil is intended during the life cycle of the test substance. Indirect exposure to the environment is unlikely, which is also indicated by the manufacturing process. In accordance with REACH, Annex IX, Section 9.2.1.4, column 2, this endpoint can be waived."*

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

According to Annex IX, Section 9.2.1.3, column 2 of the REACH Regulation, simulation testing on soil does not need to be conducted if the substance is readily biodegradable or if direct or indirect exposure of soil is unlikely. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable according to an OECD 301F (1% in 28 days) and OECD 301B (3% in 28 days).

Regarding the exposure to soil, the substance has a low water solubility (<0.05 mg/L), high partition coefficient (log Kow >6.2) and high adsorption coefficient (log Koc,soil >5), indicating high adsorptive properties. Furthermore, based on the uses reported in the technical dossier, ECHA considers that such uses are reported for which soil exposure cannot be excluded, e.g. Environmental Release Category (ERC) 9b/10a. Further, since you have not conducted an exposure assessment and/or this is not provided in the Chemical Safety Report (CSR), exposure to soil cannot be excluded. ECHA therefore considers that you have not demonstrated that soil exposure is unlikely.

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

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

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

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) Aerobic and anaerobic transformation in soil (test method EU C.23. / OECD TG 307) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.3.

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

Simulation tests performed in sediment or in soil possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product unless they are irreversibly bound by covalent bonds or incorporated into the biomass. The amount and kind of NER is operationally defined by the extraction method employed. Strong extractions methods, for example soxhlet-extraction with apolar solvents, should be used in order to qualify the remaining NER as irreversibly bound residues. You are therefore requested to justify scientifically that the extraction method you will apply is appropriate to identify non-extractable residues (NER) as residues irreversibility bound to the sediment.

In your comments you agreed that the justification provided for adaptation of the information requirements according to Annex IX, Section 9.2.1.3, column 2 ("exposure-based waiving") of the REACH Regulation did not meet the specific rules for adaptation.

You also updated your dossier (submission number: [redacted] and in this update you concluded in the PBT assessment that the registered substance is P but not vP. You also concluded that the transformation product (2,6-diisopropylaniline = DIPA) is not P nor vP.

You claim that a re-assessment of the PBT properties of the substance as contained in the most recent dossier update shows that the chemical safety assessment does not indicate any need for further investigation of degradation (i.e. soil simulation testing).

You furthermore revised the justification for adaptation of the information requirements in the updated dossier:

"In accordance to REACH, Annex IX, Section 9.2, column 2, 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. Therefore, simulation testing for biodegradation in water and sediment can be waived since it has been demonstrated that no further testing is necessary – neither for conclusions referring to the persistency of the substance nor for the environmental risk assessment.

PBT-Assessment
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.

However, conclusions on the P and vP properties of the substance could be drawn based on the available screening information. This is in compliance with ECHA REACH Guidance Chapter R.11, which states that in certain cases it may be possible to draw a conclusion "P" or "vP" based on screening information only. In terms of substance's physico-chemical/fate properties which are needed for Tier 1 exposure estimations using EUSES 2.1.2, only information on the biodegradation in water (screening tests) is necessary as model input parameter. Half-lifes in water, sediment and soil will be automatically calculated by the modelling tool if not available. Therefore, additional degradation studies are not considered necessary. Furthermore, the environmental risk assessment will address adequate RMMs to minimise emissions and subsequent exposure to the substance in order to take its persistency into account. It is therefore concluded that safe use of the substance for all environmental compartments will be achieved by using the current dataset making further refinements by results of additional simulation tests unnecessary."

ECHA notes that based on the screening studies provided the registered substance can be concluded only as potentially P, not as P (Guidance R11, table R.11-4 screening criteria).

As described in the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Section R.7.9.4 Evaluation of available information on degradation/ biodegradation: *"A negative result in a test for ready biodegradability does not necessarily mean that the chemical will not be degraded under relevant environmental conditions and persist in the environment. A failed ready biodegradability test indicates that further testing under less stringent test conditions should be considered at the next level."* Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Aerobic and anaerobic transformation in soil (test method: EU C.23./OECD TG 307).

Notes for your consideration

Before conducting the requested tests you are advised to consult the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Sections R.7.9.4 and R.7.9.6 (version 4.0, June 2017) and Chapter R.11, Section R.11.4.1.1 (version 3.0, June 2017) on PBT assessment.

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

The P assessment needs to cover the registered substance as such and the most relevant transformation products. The Registrant needs to justify his choice of the test material taking into account also the most relevant transformation products for the PBT assessment. In addition, justification needs to be provided on why some of the transformation products are not relevant for PBT assessment.

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

"Sediment simulation testing" is a standard information requirement as laid down in Annex IX, section 9.2.1.4. of the REACH Regulation for substances with a high potential for adsorption to sediment. The registered substance has low water solubility (<0.05 mg/L), high partition coefficient (log Kow >6.2) and high adsorption coefficient (log Koc, soil >5), indicating high adsorptive properties. Therefore, adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You have provided an adaptation to cover the information requirement of Annex IX, Section 9.2.1.2., simulation testing on ultimate degradation in surface waters with the justification: "*In accordance to REACH, Annex IX, Section 9.2.1.2., column 2, the study does not need to be conducted because of the low water solubility of the substance (< 0.05 mg/L, [redacted], 2008). Therefore, the study can be waived, since it is not scientifically possible to perform the test due to the properties of the test substance or because of analytical limitations of test methods.*" However, ECHA notes that regarding the information requirement for sediment simulation testing, the technical dossier does not contain an adaptation in accordance with column 2 of Annex IX, Section 9.2 or 9.2.1.4. or with the general rules of Annex XI for this standard information requirement.

According to Annex IX, Section 9.2.1.4, column 2 of the REACH Regulation, simulation testing on soil does not need to be conducted if the substance is readily biodegradable or if direct or indirect exposure of sediment is unlikely. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable in OECD 301F (1% in 28 days) and OECD 301B (3% in 28 days).

Regarding the exposure to sediment, the substance has a low water solubility (<0.05 mg/L), high partition coefficient (log Kow >6.2) and high adsorption coefficient (log Koc,soil >5), indicating high adsorptive properties. Furthermore, based on the uses reported in the technical dossier, ECHA considers that such uses are reported for which sediment exposure cannot be excluded, e.g. Environmental Release Category (ERC) 9b/10a. Further, since you have not conducted an exposure assessment and/or this is not provided in the Chemical Safety Report (CSR), exposure to sediment cannot be excluded. ECHA therefore considers that you have not demonstrated that sediment exposure is unlikely.

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

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

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

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) Aerobic and anaerobic transformation in aquatic sediment systems (test method EU C.24. / OECD TG 308) is the preferred test to cover the standard information requirement of Annex IX, Section 9.2.1.4.

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

Simulation tests performed in sediment or in soil possibly imply the formation of non-extractable residues (NER). These residues (of the parent substance and/or transformation products) are bound to the soil or to the sediment particles. NERs may potentially be re-mobilised as parent substance or transformation product unless they are irreversibly bound by covalent bonds or incorporated into the biomass. The amount and kind of NER is operationally defined by the extraction method employed. Strong extractions methods, for example soxhlet-extraction with apolar solvents, should be used in order to qualify the remaining NER as irreversibly bound residues. You are therefore requested to justify scientifically that the extraction method you will apply is appropriate to identify non-extractable residues (NER) as residues irreversibility bound to the sediment.

In your comments you agreed that the justification provided for adaptation of the information requirements according to Annex IX, Section 9.2.1.3, column 2 ("exposure-based waiving") of the REACH Regulation did not meet the specific rules for adaptation.

You also updated your dossier (submission number: [redacted] and in this update you concluded in the PBT assessment that the registered substance is P but not vP. You concluded that the transformation product (2,6-diisopropylaniline = DIPA) is not P nor vP.

You claim that a re-assessment of the PBT properties of the substance as contained in the most recent dossier update shows that the chemical safety assessment does not indicate any need for further investigation of degradation (i.e. sediment simulation testing).

You furthermore revised the justification for adaptation of the information requirements in the updated dossier similarly as in the endpoint for Soil simulation testing (Annex IX, Section 9.2.1.3.). This justification must be rejected for the same reasons (see request 1 above).

As also mentioned in the request 1, ECHA notes that based on the screening studies provided the registered substance can be concluded only as potentially P, not as P (Guidance R11, table R.11-4 screening criteria).

As described in the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Section R.7.9.4 Evaluation of available information on degradation/ biodegradation: *"A negative result in a test for ready biodegradability does not necessarily mean that the chemical will not be degraded under relevant environmental conditions and persist in the environment. A failed ready biodegradability test indicates that further testing under less stringent test conditions should be considered at the next level."*

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

Before conducting the requested tests you are advised to consult the ECHA Guidance on information requirements and chemical safety assessment, Chapter R7b, Sections R.7.9.4 and R.7.9.6 (version 4.0, June 2017) and Chapter R.11, Section R.11.4.1.1 (version 3.0, June 2017) on PBT assessment.

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

The P assessment needs to cover the registered substance as such and also the most relevant transformation products. The Registrant needs to justify his choice of the test material taking into account also the most relevant transformation products for the PBT assessment. In addition, justification needs to be provided on why some of the transformation products are not relevant for PBT assessment.

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

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

The biodegradation section in the technical dossier does not contain any information regarding the identification of degradation produces, nor it contains an adaptation in accordance with column 2 of Annex IX, Sections 9.2 or 9.2.3. or with the general rules of Annex XI for this standard information requirement.

According to Annex IX, Section 9.2.3., column 2 of the REACH Regulation, identification of degradation products is not needed if the substance is readily biodegradable. ECHA notes that based on the information in the technical dossier, the registered substance is not readily biodegradable according to an OECD 301F (1% in 28 days) and OECD 301B (3% in 28 days), as also discussed in section 5-6 above.

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

In your comments to the draft decision you agreed that adequate information on the identification of degradation products according to column 1, Section 9.2.3 of Annex IX of the REACH Regulation needs to be provided.

You proposed a tiered approach, where in the Tier 1 you suggested to: "perform scientific investigations to provide an improved analytical method and more precise water solubility. The outcome of these studies will be used for determinations referring to the following ecotoxicological endpoints."

In tier 2 you suggested to: "Based on the results of the TIER 1 approach, the registrant is willing to determine the identification of the degradation products due to hydrolysis. Furthermore, the registrant agrees to perform long-term toxicity testing on aquatic invertebrates and the bioaccumulation test in aquatic species."

In Tier 3: "After additional ecotoxicological data has been collected, an environmental risk assessment will be performed. This may indicate that no long-term fish testing is necessary anymore (if RCRs < 1). Rationale for tiered approach. A tiered approach seems to be unavoidable for the registrant for such a difficult test substance. Only with improved knowledge on analytical substance verification and a basic (reliable) dataset for the environmental risk assessment (water solubility, degradation products due to hydrolysis), test designs for the requested long-term toxicity testing on aquatic invertebrates and bioaccumulation in aquatic species can be developed."

ECHA emphasises that any testing strategy or adaptation is the Registrant's responsibility. ECHA notes that guidance on how degradation/transformation products should be considered for various standard information requirements is given in different sections of ECHA's Guidance on Information Requirements and Chemical Safety assessment (for e.g. Chapter R.7b, Version 4.0, June 2017; Chapter R.11, Version 3.0June 2017).

If you decide to adapt the testing requested according to the specific rules outlined in Annexes VI to X and/or according to general rules contained in Annex XI of the REACH Regulation, to ensure compliance with this standard 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.

ECHA notes your thorough analysis of these investigations of the substance's hydrolytic properties may allow you to conclude on the non-persistence of the registered substance. In the event that non-persistence of the substance in all relevant compartments can be shown and degradation products concluded not to be PBT/vPvBs the requested simulation testing might become unnecessary, as instructed by ECHA Guidance on information requirements and chemical safety assessment, Chapter R.11, Section R.11.4.1.1 (version 3.0, June 2017), "*Hydrolysis may proceed effectively in aquatic, sediment and soil compartments but it is however noted that there are substances reaching rapid hydrolysis rates which are well known to be persistent in soil and/or sediment, e.g. endosulfan. Therefore, rapid hydrolysis rates cannot alone lead to concluding that a substance is not persistent. Test results showing rapid hydrolysis rates always need to be evaluated carefully in context with other information on the substance, such as partitioning and ionogenic properties both of which may significantly influence the extent and strength of sorption to soil and sediment. Hydrolysis also needs to be consistently rapid across the range of environmentally relevant pH. To provide confidence in the hydrolysis results, analytical data identifying metabolites to provide a mass balance are also needed. These both demonstrate that primary degradation has occurred, and allow subsequent PBT assessment of the degradants*".

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

Identification of the degradation products (Annex IX, Section 9.2.3.) by using an appropriate and suitable test method, as explained above in this section.

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

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

You proposed to adapt these information requirements on bioaccumulation in aquatic species of the substance by providing results obtained from the application of quantitative structure activity relationship models ((Q)SARs). You provided QSAR predictions for the registered substance, *bis(2,6 -diisopropylphenyl)carbodiimide* (CDI), and also for the relevant hydrolysis product *2,6 -diisopropylaniline* (DIPA), using EPi Suite (BCFBAF WIN v.3.01). In particular, you reported a Bioconcentration Factor (BCF) for CDI of 1912 L/kg ww (regression-based estimate), and a BCF for DIPA of 58.23 L/kg ww (regression-based estimate), thus concluding that relevant bioaccumulation of the registered substance and of the hydrolysis product DIPA is not to be expected.

According to Annex XI, Section 1.3. of the REACH Regulation the results of (Q)SARs may be used instead of testing when the following conditions are met:

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

You did not provide the adequate and reliable documentation of the applied model referred to under the fourth bullet point above. Without such documentation ECHA is not in a position to assess whether the other conditions outlined in the first three bullet points are fulfilled. As you have not demonstrated that the conditions of the adaptation of Annex XI, Section 1.3. of the REACH Regulation are fulfilled, ECHA cannot accept the adaptation.

For the adaptation to be acceptable, you would have to provide the above mentioned documentation and you would have to demonstrate that the first three conditions for applying the proposed adaptation are fulfilled. The general form of the (Q)SAR Model Reporting Format (QMRF) and (Q)SAR Prediction Reporting Format (QPRF), are described in the ECHA Guidance on information requirements and chemical safety assessment Chapter R.6: (Q)SARs and grouping of chemicals (ECHA, May 2008). Under REACH, reporting formats can be submitted to ECHA as attached files in an IUCLID dossier.

As the conditions for adapting the information requirements in accordance with Annex XI, Section 1.3. of the REACH Regulation have not been fulfilled and no other information is available in the dossier for the endpoints in question, ECHA concludes that there are information gaps and that it is necessary to provide information for the endpoint in order to bring the registration dossier into compliance with relevant information requirements.

Furthermore, the reliability of the prediction for CDI generated with the BCF Meylan model (regression-based estimate) is questionable, since the training set of the model does not contain carbamides. The same applies to the Arnot-Gobas 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 3.0,June 2017) bioaccumulation in fish: aqueous and dietary exposure (test method EU C.13. / OECD TG 305) is the preferred test to cover the standard information requirement of Annex IX, Section 9.3.2. ECHA Guidance defines further that results obtained from a test with aqueous exposure can be used directly for comparison with the B and vB criteria of Annex XIII of REACH Regulation and can be used for hazard classification and risk assessment. Comparing the results of a dietary study with the REACH Annex XIII B and vB criteria is more complex and has higher uncertainty. Therefore, the aqueous route of exposure is the preferred route and shall be used whenever technically feasible. If you decided to conduct the study using the dietary exposure route, you shall provide scientifically valid justification for your decision. Data obtained from a dietary study will also need to be used to estimate BCF values.

In your comments you agreed that the reliability of the submitted QSAR-predictions is questionable. You agreed to perform the bioaccumulation test in aquatic species and specified that results based on further scientific investigations (i.e. water solubility and identification of degradation products due to hydrolysis) are crucial for developing an appropriate test design for bioaccumulation testing.

In your comments on the draft decision you agreed with the principle of the request and indicated that you will design the test based on further scientific investigations (i.e. water solubility and identification of degradation products due to hydrolysis).

ECHA emphasises that any testing strategy or adaptation is the Registrant's responsibility.

ECHA notes that guidance on how degradation/transformation products should be considered for various standard information requirements is given in different sections of ECHA's Guidance on Information Requirements and Chemical Safety assessment (for e.g. Chapter R.7b, Version 4.0, June 2017; Chapter R.11, Version 3.0, June 2017).

If you decide to adapt the testing requested according to the specific rules outlined in Annexes VI to X and/or according to general rules contained in Annex XI of the REACH Regulation, to ensure compliance with this standard 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.

As stated above in request 3, a thorough analysis of these investigations of the substance's hydrolytic properties may allow you to conclude on the non-persistence of the registered substance. Furthermore before conducting testing, you are advised to consult the ECHA Guidance on the information requirements and chemical safety assessment (version 3.0, June 2017), Chapter R.11. PBT/vPvB assessment, to consult the PBT assessment for Weight-of-Evidence determination and the integrated testing strategy for bioaccumulation assessment, in particular concerning relevant constituents, impurities, additives and degradation/transformation products. Also, you need to carefully consider the potential formation of stable degradation products with PBT/vPvB properties. Moreover, other than the PBT/vPvB assessment, other needs of the CSA (e.g. environmental hazard assessment, exposure assessment) for information on bioaccumulation of the substance has to be also considered by you.

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

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

Notes for your consideration

Before conducting the above test, you are advised to consult the ECHA *Guidance on information requirements and chemical safety assessment* (version 3.0, June 2017), Chapter R.11.4. and Figure R.11-4 on the PBT assessment for further information on the integrated testing strategy for the bioaccumulation assessment of the registered substance. You should revise the PBT assessment when information on bioaccumulation is available.

The B assessment needs to cover the registered substance as such and the most relevant transformation products. The Registrant needs to justify his choice of the test material taking into account also the most relevant transformation products for the PBT assessment. In addition, justification needs to be provided why some of the transformation products are not relevant for PBT assessment.

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

"Long-term toxicity testing on aquatic invertebrates" is a standard information requirement as laid down in Annex IX, Section 9.1.5. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

You proposed to adapt these information requirements on long-term toxicity testing on aquatic invertebrates of the substance by providing results obtained from the application of quantitative structure activity relationship models ((Q)SARs). You provided QSAR predictions for the registered substance with ECOSAR v1.00 (EPIWIN software by US-EPA), Chronic Value for daphnids: 0.000175 mg/L. In addition, you provided the following justification: "*The prediction for long-term toxicity for aquatic organisms of the substance bis(2,6-diisopropylphenyl)carbodiimide was determined by the computer program ECOSAR v1.00 (EPIWIN software) by US-EPA ([redacted] 2011). The program uses an extensive set of structure-activity relationships (SARs) to estimate the toxicity of chemicals discharged to water. For daphnids a Chronic Value (ChV) of 0.000175 mg/L was predicted. No GLP criteria are applicable for the usage of this tool, but due to the fact that it is a scientifically accepted calculation method the estimations performed are reliable with restrictions, but cannot be used for the chemical safety assessment.*"

According to Annex XI, Section 1.3. of the REACH Regulation the results of (Q)SARs may be used instead of testing when the following conditions are met:

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

- adequate and reliable documentation of the applied model is provided.

You did not provide the adequate and reliable documentation of the applied model referred to under the fourth bullet point above. Without such documentation ECHA is not in a position to assess whether the other conditions outlined in the first three bullet points are fulfilled. As you have not demonstrated that the conditions of the adaptation of Annex XI, Section 1.3. of the REACH Regulation are fulfilled, ECHA cannot accept the adaptation.

For the adaptation to be acceptable, you would have to provide the above mentioned documentation and to demonstrate that the first three conditions for applying the proposed adaptation are fulfilled. The general form of the (Q)SAR Model Reporting Format (QMRF) and (Q)SAR Prediction Reporting Format (QPRF), are described in the ECHA Guidance on information requirements and chemical safety assessment Chapter R.6: (Q)SARs and grouping of chemicals (ECHA, May 2008). Under REACH, reporting formats can be submitted to ECHA as attached files in an IUCLID dossier.

As the conditions for adapting the information requirements in accordance with Annex XI, Section 1.3. of the REACH Regulation have not been fulfilled and no other information is available in the dossier for the endpoints in question, ECHA concludes that there are information gaps and that it is necessary to provide information for the endpoint in order to bring the registration dossier into compliance with relevant information requirements.

Furthermore, the predictions were only ran on the parent molecule. The calculated log Kow of CDI exceed the maximum for the model, so it cannot be considered reliable. In addition, the model for Neutral organic substances was used in the calculations. For these cases, ECOSAR warns:

Estimates provided below use the Neutral Organics QSAR equations which represent baseline toxicity potential (minimum toxicity) assuming a simple non-polar narcosis model. Without empirical data on structurally similar chemicals, it is uncertain if this substance will present significantly higher toxicity above baseline estimates.

A look at the training set of the model showed that no carbamides are present, so the actual toxicity of the parent might be even higher than calculated.

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

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

According to ECHA *Guidance on information requirements and chemical safety assessment, Chapter R.7b* (version 4.0, June 2017) *Daphnia magna* reproduction test (test method EU C.20. / OECD TG 211) is the preferred test to cover the standard information requirement of Annex IX, Section 9.1.5.

In your comments you agreed that the reliability of the submitted QSAR-predictions is questionable. You agreed to perform long-term toxicity testing on aquatic invertebrates after performing scientific investigations to provide an improved analytical method and more precise water solubility.
Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, you are requested to submit the following information derived with the registered substance subject to the present decision: Daphnia magna reproduction test (test method: EU C.20./OECD TG 211).

Notes for your consideration

According to ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), Chapter R7b (Section R.7.8.5., including Figure R.7.8-4) if based on acute aquatic toxicity data neither fish nor invertebrates are shown to be substantially more sensitive, long-term studies may be required on both. In such case, according to the integrated testing strategy, the *Daphnia* study is to be conducted first. If based on the results of the long-term *Daphnia* study and the application of a relevant assessment factor, no risks are observed (PEC/PNEC<1), no long-term fish testing may need to be conducted. However, if a risk is indicated, the long-term fish study needs to be conducted.

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

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

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

You proposed to adapt these information requirements on long-term toxicity testing on fish by providing results obtained from the same QSAR application model as for the long-term toxicity testing on aquatic invertebrates. Therefore, for the same reasons and further considerations outlined under request 9 above, your adaptation of the information requirement cannot be accepted.

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

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

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

Moreover, the FELS toxicity test is preferable for examining the potential toxic effects of substances which are expected to cause effects over a longer exposure period, or which require a longer exposure period of time to reach steady state (ECHA *Guidance Chapter R7b,* version 4.0, June 2017).

In your comments you agreed that the information provided on this endpoint does not meet the information requirements since the submitted QSAR-predictions are of questionable reliability. You proposed a tiered approach for testing ecotoxicological endpoints. This proposed approach also foresees to conduct long -term toxicity testing on fish in case a revised chemical safety assessment indicates further need for testing.

ECHA highlights that this tiered approach is already addressed in the Notes for consideration: "If based on the results of the long-term Daphnia study and the application of a relevant assessment factor, no risks are observed (PEC/PNEC<1), no long-term fish testing may need to be conducted. However, if a risk is indicated, the long-term fish study needs to be conducted."

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

Notes for your consideration

Before conducting any of the tests mentioned above in points 9-10 you shall consult the ECHA *Guidance on information requirements and chemical safety assessment (version 4.0, June 2017)*, Chapter R7b, Section R.7.8.5 to determine the sequence in which the aquatic long-term toxicity tests are to be conducted and the necessity to conduct long-term toxicity testing on fish.

According to ECHA *Guidance on information requirements and chemical safety assessment* (version 4.0, June 2017), Chapter R7b (Section R.7.8.5., including Figure R.7.8-4), if based on acute aquatic toxicity data neither fish nor invertebrates are shown to be substantially more sensitive, long-term studies may be required on both. In such case, according to the integrated testing strategy, the *Daphnia* study is to be conducted first. If based on the results of the long-term *Daphnia* study and the application of a relevant assessment factor, no risks are observed (PEC/PNEC<1), no long-term fish testing may need to be conducted. However, if a risk is indicated, the long-term fish study needs to be conducted.

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

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 6 October 2016.

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

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

In your comments, you have agreed to self-classify the substance as Repr. 1B, H360F and STOT RE 1 as requested by ECHA. Due to this, ECHA exceptionally agreed that you could submit an updated dossier.

You updated your registration with new submission number [redacted] on 10 February 2017. In your update, you have self-classified the substance as Repr. 1B, H360F and STOT RE 1.

Given the exceptional circumstances, ECHA took into account your update of 10 February 2017 and your comments on the draft decision. As a result, ECHA has removed the following draft decision requests: Classification and labelling: Apply classification and labelling on the registered substance for reproductive toxicity or provide a justification for not classifying; Classification and labelling: Apply classification and labelling on the registered substance for specific target organ toxicity repeated dose or provide a justification for not classifying; Extended one-generation reproductive toxicity study; Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method: EU B.31./OECD TG 414) in a first species (rat or rabbit), oral route with the registered substance; ECHA has modified Appendix 1 for the following draft decision requests: Soil simulation testing; Sediment simulation testing; Identification of degradation products; Bioaccumulation in aquatic species; Long-term toxicity testing on aquatic invertebrates; Long-term toxicity testing on fish with the registered substance.

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

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

As no amendments were proposed, ECHA took the decision according to Article 51(3) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

1) The substance subject to the present decision is provisionally listed in the Community rolling action plan (CoRAP) for start of substance evaluation in 2018.

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

3) Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.

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

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

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

5) ECHA reminds you that Article 14(4) of the REACH Regulation requires an exposure assessment if there is classification under any of the hazard classes identified.

   In your dossier, there is currently no environmental exposure assessment on the basis that the substance is not classified for the environment; however, if the results of the test requested under this decision trigger such classification, exposure assessment would be required.

   In addition, because the registered substance is classified for human health, an environmental exposure assessment will also be required if an environmental hazard is detected below the highest recommended concentration/doses tested.