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Helsinki, 17 April 2018

Substance name: Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene
EC number: 270-128-1
CAS number: 68411-46-1
Date of Latest submission(s) considered[1]: 22 March 2017
Decision/annotation number: Please refer to the REACH-IT message which delivered this communication (in format SEV-D-XXXXXXXXXX-XX-XX/F)
Addressees: Registrant(s)[2] of Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene (Registrant(s))

DECISION ON SUBSTANCE EVALUATION

Based on Article 46(1) of Regulation (EC) No 1907/2006 (the 'REACH Regulation'), you are requested to submit the following information on one isomer of the constituent Ditertbutyldiphenylamine (hereafter named DTBDA) ppDTBDA **or** poDTBDA[3] of the registered substance as further specified in Appendix 1:

1. Physico-chemical properties
   1.A: Water solubility (OECD 105) (using the column elution method)

   and

   1.B: Partition Coefficient (1-Octanol/Water): Slow-Stirring Method (OECD 123) or HPLC Method (OECD 117).

2. Simulation testing on ultimate degradation in surface water; test method: Aerobic mineralisation in surface water - simulation biodegradation test at 12°C, EU C.25./OECD 309, pelagic test – without additional suspended solids/sediment, as specified in Appendix 1.

If the results from requirement 2 show that the substance is not P/vP in the tested compartment and these results are sufficient to conclude on persistence in other environmental compartments, no additional simulation tests will be needed. If a concern on the persistence in some of the compartments remains, ECHA can consider whether further simulation testing needs to be requested in future SEV decisions.

If the results from requirement 2 allows to conclude that the registered substance is

[1] This decision is based on the registration dossier(s) at the end of the 12 month evaluation period.
[2] The terms Registrant(s), dossier(s) or registration(s) are used throughout the decision, irrespective of the number of registrants addressed by the decision.
[3] [redacted]

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persistent (P) or very persistent (vP) according to Annex XIII of the REACH Regulation the following test using ppDTBDA **or** poDTBDA is required:

3. Bioaccumulation in aquatic species; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD 305, [aqueous exposure] as specified in Appendix 1.

If the results from requirement 2 and, if required, 3 allow to conclude that the substance is persistent and bioaccumulative (P/B), or very persistent and bioaccumulative (vP/B), or persistent and very bioaccumulative (P/vB) according to Annex XIII of the REACH Regulation, the following toxicity tests using ppDTBDA **or** poDTBDA are required:

4. Toxicity testing

4.A: Long-term toxicity testing on aquatic invertebrates; test method: *Daphnia magna* reproduction test, EU C.20./OECD 211 specified in Appendix 1;

and

4.B: Growth inhibition study aquatic plants; test method: Algae, growth inhibition test, EU C.3./OECD 201 as specified in Appendix 1.

If the results from requirements 4.A and 4.B do not allow to conclude that the registered substance is toxic (T) according to Annex XIII of the REACH Regulation, the following toxicity test using ppDTBDA **or** poDTBDA is required:

4.C: Long-term toxicity testing on fish; test method: Fish, early-life stage (FELS) toxicity test, OECD 210 as specified in Appendix 1.

You shall provide an update of the registration dossier(s) containing the requested information, including robust study summaries, full study reports and, where relevant, an update of the Chemical Safety Report by the following timelines. The full study report must be submitted for all studies under requests 1, 2, 3 and 4 to allow the evaluating MSCA to analyse the raw data and consider study details to conclude on the scientific merits of the studies and the interpretation of the results. The deadlines take into account the time that you, the Registrant(s), may need to agree on who is to perform any required tests, and they have been set to allow for sequential testing.

- The information required according to points 1.A and 1.B shall be generated and provided by **24 April 2019**.

- The information required according to point 2 shall be generated and provided by **26 April 2021**.

If the results of requirement 2 demonstrate that the registered substance does not fulfil the P or vP criterion (according to Annex XIII of the REACH Regulation), no further testing according to information requests 3 and 4 are required.

- Where applicable, the information required according to point 3 shall be generated and provided by **24 January 2022**.

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If the results of requirements 2 and 3 demonstrate that the registered substance either does not fulfil the B or vB criterion, or fulfils the vP and vB criterion (according to Annex XIII of REACH), no further testing according to information requests 4 A-C is required.

- Where applicable, the information required according to point 4.A and 4.B shall be generated and provided, by **24 July 2023**.

If the results of requirements 4.A and 4.B demonstrate that the registered substance fulfils the T criterion (according to Annex XIII of REACH), no further testing according to information request 4.C is required.

- Where applicable, the information required according to point 4.C shall be generated and provided, by **24 July 2024**.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2. Further information, observations and technical guidance as appropriate are provided in Appendix 3. Appendix 4 contains further technical information used to support the reasons of the decision. Appendix 5 contains a list of registration numbers for the addressees of this decision. This appendix is confidential and not included in the public version of this decision.

Who performs the testing?

Based on Article 53 of the REACH Regulation, you are requested to inform ECHA who will carry out the studies on behalf of all Registrant(s) within 90 days. Instructions on how to do this are provided in Appendix 3.

Appeal

You can appeal this decision 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[4] by Leena Ylä-Mononen, Director of Evaluation

[4] 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

Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene (hereafter named the 'registered substance') was nominated for the Community Rolling Action Plan because it fulfils the screening criteria for persistence and bioaccumulation as defined in Annex XIII of the REACH Regulation.

If the registered substance is eventually confirmed to meet the criteria for PBT/vPvB, the evaluating Member State Competent Authority (MSCA) will assess the need for appropriately revised Risk Management Measures (RMM) under the REACH Regulation or any other relevant legislation. For a PBT/vPvB substance, this would typically be inclusion in the candidate list as a Substance of Very High Concern (SVHC) and authorisation under Title VII of the REACH Regulation.

As stated in Chapter R.11 (PBT Assessment) of ECHA's Guidance on information requirements and chemical safety assessment (June 2017), the PBT/vPvB assessment must consider persistence, bioaccumulation and toxicity against each respective criterion of Annex XIII of the REACH Regulation in order to conclude on the properties of a substance and its relevant constituents, impurities, additives and transformation/degradation products.

Based on the evaluation of all relevant information submitted on the registered substance and other relevant available information, ECHA concludes that further information is required in order to enable the evaluating MSCA to complete the evaluation of whether the substance constitutes a risk to the environment. The evaluating MSCA will subsequently review the information submitted by you and evaluate if further information should be requested in order to clarify the concern for PBT-properties.

All available data on persistence, bioaccumulation and toxicity of the registered substance were assessed in a weight-of-evidence approach by the evaluating MSCA. The registered substance is a substance of unknown or variable composition, complex reaction products or Biological materials (UVCB) containing eleven identified constituents at well-defined concentration ranges. Besides Diphenylamine and 2,4,4-Trimethyl-pent-2-ene as starting material, the registered substance consists of mono-, di- and tri-alkylated diphenylamine isomers. The alkyl chains, tert-butyl and/or tert-octyl, were substituted in para position (major part) or in ortho position (minor part) of the nitrogen atom of both aromatic rings. With regard of their molecular weight, para-para-, para-ortho- and ortho-ortho-isomers (para/ortho-isomers) were clustered into Group A, B and C (see Annex 4, Table 1). With a typical concentration of around [redacted]%, Group A has the highest percentage amount in the UVCB substance (Group B around [redacted]%, Group C around [redacted]%). Group A consists of the para/ortho-isomers of Monotertoctyldiphenylamine and DTBDA with a molecular weight of 281.44 g/mol.

Due to the well-defined composition of the registered substance regarding its constituents and their typical concentration range in the UVCB substance, assessment of the registered substance shall be performed by the consideration of one constituent of most relevance regarding potentially (v)P, (v)B and T properties according to screening level information. QSAR estimations provided by you and the evaluating MSCA's calculations regarding potentially PBT properties for nine relevant para/ortho alkylated diphenylamine isomers of the registered substance are indicated in Appendix 4 (Table 1).

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In your comments, you note the registered substance is a member of the 'Substituted Diphenylamines' group in a collaborative approach pilot project initiated by ECHA where France is the lead MSCA. The evaluating MSCA appreciates this collaborative approach and has offered future collaboration to the MSCA of France and ECHA.

Furthermore, in your comments, you also note that the registered substance is currently being assessed by Environment and Climate Change Canada, which published a draft screening assessment on 14 substituted diphenylamines (including the registered substance) in December 2016 with following conclusion concerning the Canadian Environmental Protection Act (CEPA, 1999), section 64:

'Considering all available lines of evidence presented in this draft screening assessment, there is low risk of harm to organisms and the broader integrity of the environment from the fourteen SDPAs considered in this assessment. It is proposed to conclude that the fourteen SDPAs do not meet the criteria under paragraphs 64(a) or (b) of CEPA as they are not entering the environment in a quantity or concentration or under conditions that have or may have an immediate or long-term harmful effect on the environment or its biological diversity or that constitute or may constitute a danger to the environment on which life depends. Based on the available information on their potential to cause harm to human health, it is proposed that the fourteen SDPAs considered in this assessment do not meet the criteria under paragraph 64(c) of CEPA as they are not entering the environment in a quantity or concentration or under conditions that constitute or may constitute a danger in Canada to human life or health. It is proposed to conclude that the fourteen SDPAs considered in this assessment do not meet any of the criteria set out in section 64 of CEPA. ....'

ECHA is aware of the ongoing assessment of the registered substance by Environment and Climate Change Canada and the published draft screening assessment. However, ECHA also notes that the criteria defined within paragraph 64 of the Canadian Environmental Protection Act (CEPA, 1999) are not comparable to the criteria set out in the Annex XIII of the REACH regulation.

Determination of the most relevant constituent regarding PBT properties

Based on the available screening level information on persistency, bioaccumulation and toxicity of all relevant constituents of the registered substance, some constituents have potential PBT properties based on estimations regarding log P_{ow}, ready biodegradability and long-term toxicity (Appendix 4, Table 1).

On the basis of the bioaccumulation potential (BCF values estimated by EPISuite Version 4.11), ECHA considers that the constituents of Group A (para/ortho-isomers of DTBDA and Monotertoctyldiphenylamine) are the most relevant constituents of the registered substance with regards to the PBT assessment.

Concerning the bioaccumulation potential of both constituents of Group A, para/ortho-isomers of DTBDA show approximately the same bioaccumulation potential regarding the regression based BCF (12500 L/kg and 11700 L/kg). However, regarding the Arnot-Gobas model, DTBDA shows a substantially higher estimated BCF value (6761 L/kg) compared to para/ortho-isomers of Monotertoctyldiphenylamine (2667 L/kg). Furthermore, based on models estimating chemical structure it can be expected that para/ortho-isomers of Monotertoctyldiphenylamine have a higher average molecular diameter leading to a certain steric hindrance when passing membrane. Thus, it is expected that para/ortho-isomers of Monotertoctyldiphenylamine may have a lower

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bioaccumulation potential. Therefore, according to the evaluation strategy mentioned above, para-para-, para-ortho- and ortho-ortho-isomers of DTBDA are considered as the most relevant constituent with respect to potential PBT properties based on screening level information.

QSAR estimations further indicate that the water solubility of DTBDA (S_w=0.014 mg/L) allows maintaining stable aquatic concentrations required for a bioaccumulation study with aquatic exposure and toxicity testing. According to you, DTBDA consist of four isomers: para-para; para-ortho (two rings); ortho-ortho; para-ortho (one ring). For the para-para and para-ortho (two rings) isomers named [redacted] (CAS [redacted]) (ppDTBDA) and [redacted] (CAS [redacted]) (poDTBDA) academia on synthetic route are available enabling the synthesis of the single isomers for purpose of testing. Thus, testing ppDTBDA **or** poDTBDA as para-para and para-ortho (two rings) isomers of the constituent DTBDA is required to clarify if this isomer meets the P, B and T criteria according to Annex XIII of the REACH Regulation and to decide whether the registered substance has PBT or vPvB properties. Based on the results it has to be concluded if further testing of other constituents of the registered substance is necessary.

ECHA notes that, based on their physico-chemical properties, several constituents of the registered substance may be considered as relevant with regards to the PBT assessment. On this basis, the standard approach would be to investigate the potential PBT properties of constituents of relevance for the PBT assessment, at the same time. However, ECHA notes that in your comments on the proposals for amendments (PfAs), you highlighted that there would be technical difficulties with performing the requested tests on more than one constituent at the same time.

Consequently, on the basis of the specific technical difficulties that you have indicated for this substance, the present decision requests testing on only one constituent of the registered substance. However, the evaluating MSCA will review the information generated by the studies requested in the present decision and determine whether further testing of other constituents of the registered substance is necessary to clarify the PBT concern.

Consideration of Registrants' comments

In your comments, you agree based on the available data to test the para/ortho isomers of DTBDA as the most relevant constituent concerning potential PBT, vPvB properties. However, you questioned the statement that eight of nine constituents would have potential PBT properties and most of the constituents would be toxic. You state that considering the QSAR estimations with ECOSAR, only the estimations of three of the nine constituents (monotertoctyldiphenylamine, DTBDA, monotertbutyldiphenylamine) show chronic aquatic toxicity below the saturation concentration according to ECOSAR v1.11 for neutral organics.

ECHA agrees that the ECOSAR v1.11 calculations for the constituents of the registered substance with a log P_{ow} > 10 are above the cut-off limit (Chapter R.11 of ECHA's Guidance on information requirements and chemical safety assessment, June 2017), as there are no neutral organics in the model training set of ECOSAR v1.11 above this log P_{ow} value. However, a log P_{ow} > 10 does not exclude that a substance might fulfil the toxicity criterion of Annex XIII. As no reliable screening information for constituents with a very high log P_{ow} is available, the draft decision was amended to indicate that some

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constituents of the registered substance have potential PBT properties based on estimations regarding log Pow, ready biodegradability and long-term toxicity.

You also state that experimental data on aquatic toxicity available for one of the constituents (ditertoctyldiphenylamine) shows no adverse effects at saturation. ECHA agrees that available experimental data on the aquatic toxicity of Ditertoctyldiphenylamine shows no adverse effects at saturation. However, Ditertoctyldiphenylamine is a poorly soluble substance and no data regarding long-term effects on fish or daphnia are available. Based on the available data, no definitive conclusion can be drawn if Ditertoctyldiphenylamine fulfils the T-criterion of Annex XIII.

Furthermore, you note that ECHA did not consider the QSAR estimations derived with OASIS Catalogic BCF Baseline model v2.09 and the applied mitigating factors which were additionally submitted by you including the QPRF - and QMRF- documents. The molecular structures of the submitted estimations for the constituents are in the structural, mechanistic and parametric domain of the model and therefore considered reliable. For structures 3, 8 and 9 shown in Table 1 of Appendix 4 you performed additional QSAR estimations with OASIS Catalogic BCF Baseline model v2.09 and indicated that the QPRF- and QMRF-documents can be provided upon request.

ECHA agrees that no QSAR estimations derived with OASIS Catalogic BCF Baseline model v2.09 were used for the identification of the most relevant constituent of Group A with regard to the PBT-assessment. According to Chapter R.11 (PBT Assessment) of ECHA's Guidance on information requirements and chemical safety assessment (June 2017), a Log P_{ow} > 4.5 has been established as a screening criterion for the PBT and vPvB assessment. Both constituents of Group A (para/ortho-isomers of DTBDA and monotertoctyldiphenylamine) show log P_{ow} values > 4.5 indicating potential bioaccumulative properties. Information on BCF values estimated by EPISuite Version 4.11 are only used to refine the B-assessment and to decide which of both potential bioaccumulative constituents of Group A are the most relevant regarding PBT-properties. According to the QSAR estimations derived with OASIS Catalogic BCF Baseline model v2.09 both constituents of Group A (para/ortho-isomers of DTBDA and monotertoctyldiphenylamine), show BCF values below 2000 L/kg. Using EPISuite Version 4.11, BCF values of both constituents are greater than 2000 L/kg. Calculated Log P_{ow} values of para/ortho-isomers of DTBDA and monotertoctyldiphenylamine are as follows: 7.05 and 7.11. According to Chapter R.7C of ECHA's Guidance on information requirements and chemical safety assessment (June 2017) it should be noted that BCF models tend to have large uncertainty ranges and predictions for substances with log P_{ow} >6 need careful consideration.

Regarding the synthesis of the most relevant constituent, you state that, as indicated by the name of the registered substance "Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene", the scope of the reaction is not primarily to synthesize DTBDA, but to receive a reaction product preferably tertiary octylated. Both, C4 and/or C8 groups of constituents are found in "Group A" and are most probably present in a significant amount in the UVCB substance, but you cannot assign neither exact structures, nor the related content so far. Furthermore, the chemical process you use and know is not optimized to generate this group of isomers forming the requested constituent DTBDA with a quality and purity as requested for a constituent-related examination of its PBT properties. Consequently, you proposed as a first step in the process of generating a PBT assessment of this constituent DTBDA, to work out a corresponding manufacturing process and agree with the evaluating MCSA on the composition of the test item to be examined further.

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The evaluating MSCA agrees that the scope of the reaction used during the manufacture of the registered substance is not primarily to synthesize DTBDA, but to receive a reaction product preferably higher octylated. DTBDA is di butylated and it seems reasonable that the synthetic route used to synthesise the registered substance is not appropriate to only synthesise para/ortho-isomers of DTBDA, which should be used as test item. Consequently, the evaluating MSCA agrees to your proposal to discuss the manufacturing process with you.

Proposals for amendment by other MSCAs and ECHA

PfAs were submitted by two MSCAs regarding the test material. One MSCA suggested to test the whole fraction of constituents of MW = 281.3 g/mol (isomers of DTBDA and isomers of Monotertoctyldiphenylamine, group A). The decision was not amended for the following reasons: ECHA recognizes that the estimated log K_{ow} values of both isomers of monotertoctyldiphenylamine and isomers of DTBDA are nearly similar. Based on models estimating chemical structure it can be expected that isomers of monotertoctyldiphenylamine have a higher average molecular diameter leading to a certain steric hindrance when passing the membrane. Thus, it is expected that these isomers of monotertoctyldiphenylamine may have a lower bioaccumulation potential. For the assessment of the UVCB substance, the "Known constituent approach" was chosen. This approach can be applied when a substance is known to contain specific constituents at relevant concentrations, these constituents are suspected based on available information to represent the worst case of the (v)P, (v)B and T properties of all constituents of the substance, and these specific constituents can be isolated or separately manufactured or otherwise acquired for the purpose of testing. The substance can be deemed as "not PBT/vPvB" if none of the relevant constituents individually is PBT or vPvB. This does not mean that all known constituents need to be tested but step-wise assessment and testing is crucial for focussing on the known constituents which represent the worst case in relation to the PBT/vPvB properties among all constituents of the substance. If one or more of the constituents are proven to fulfil either the vPvB or PBT criteria, the entire (registered) substance must be concluded as PBT and/or vPvB (Chapter R.11 of ECHA's Guidance on information requirements and chemical safety assessment, June 2017). The registered UVCB substance contains eleven well defined constituents. Based on screening level information DTBDA is regarded as most relevant constituent regarding PBT-properties. According to your estimations, this constituent could be manufactured separately. Testing the whole fraction of constituents of MW = 281.3 g/mol (isomers of DTBDA and isomers of monotertoctyldiphenylamine) in the requested tests on persistency, bioaccumulation and toxicity makes it impossible to distinguish which of the both identified constituents of the UVCB substance have PBT properties. However, within the chosen assessment approach for the PBT assessment of the UVCB substance it is mandatory to prove if one or more constituents fulfil either the vPvB or PBT criteria.

In addition, the MSCA suggested to apply a testing strategy considering all three fractions of MW = 225.2 g/mol, MW = 281.3 g/mol and MW = 337.4 g/mol. The decision was not amended for the following reasons: For DTBDA actually five sequential testing requests (OECD 309, OECD 305, OECD 201, OECD 211 and OECD 210) are included in the decision, because no individual data on this constituent are available, which were needed for assessing the UVCB substances using the "Known constituent approach". If a test strategy considering all three fractions was applied and the constituent isomers of DTBDA of fraction MW = 281.3 g/mol did not fulfil PBT-criteria, respectively the five test requests would have to be performed for i) isomers of Monotertoctyldiphenylamine of fraction MW = 281.3 g/mol, ii) constituents of fraction MW = 225.2 g/mol as well as for

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iii) constituents of fraction MW = 337.4 g/mol because no individual data on these constituents are available for assessing the UVCB substance with the "Known constituent approach". As it is expected that DTBDA of MW fraction = 281.3 g/mol represents the worst case with respect to P, B and T it is thus very unlikely that DTBDA and thereby the whole substance would be considered as non PBT/vPvB.

Another PfA made by a MSCA suggested to include the option for a further PBT related follow-up testing of the other constituents of the registered substance if this seems to be appropriate based on the results of the required tests. This is reflection in the decision.

Comments from the Registrant(s) on the proposals for amendment

In your comments on PfAs you disagreed to the PfA proposing to test the whole fraction of constituents of MW = 281.3 g/mol.

You ruled out that para/ortho isomers of DTBDA consists of four different isomers and for only two academia on a synthetic route are available: [redacted] (CAS [redacted]) (ppDTBDA) and [redacted] (CAS [redacted]) (poDTBDA). For the other two the synthetic route has to worked out. You provided data on log Pow and estimated BCF-values of ppDTBDA and poDTBDA indicating that both isomers have an equal bioaccumulation potential. You proposed to test one of the two known representative structures from the fraction MW 281 g/mol. This is technically more feasible, the results are easier to interpret and also easier to use for other co-registrants which might have a different composition of the MW 281 g/mol fraction.

1. Physico-chemical properties

The Concern(s) identified and why new information is needed

Requirements regarding physico-chemical properties (1.A and 1.B) were not included in the first draft decision. A proposal for amendment (PfA) was submitted by one MSCA suggesting to request a water solubility test (OECD TG 105) and a test to determine log K_{ow} (OECD TG 123 or TG 117) before starting the PBT strategy. After evaluating the PfA and your comments on the initial draft decision and the PfA, ECHA decided to include these tests as separate requirements.

The registration dossiers contain a water solubility test on the registered UVCB-substance. You conclude from this test that the water solubility of the UVCB substance is 2 mg/L. For the single constituents of the registered substance only QSAR estimations are provided by you and the evaluating MSCA's calculations are available indicating that DTBDA has a water solubility of 0.014 mg/L. No experimental data on water solubility for para-para and para-ortho (two rings) isomers of DTBDA, ppDTBDA and poDTBDA, are available.

The registration dossiers contain QSAR estimations provided by you on log P_{ow} values for group A, B, C and [redacted]. You conclude from this data that the log P_{ow} of the UVCB substance is ≥5 at 25°C. For Group A which includes DTBDA the estimated log P_{ow} is 7.11 at 25°C. No experimental data on log P_{ow} of para-para and para-ortho (two rings) isomers of DTBDA, ppDTBDA and poDTBDA, are available.

Information on water solubility and log P_{ow} are essential endpoints for correct bioaccumulation and toxicity testing, but also relevant for simulation degradation testing.

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As indicated above, the constituent DTBDA is regarded as the most relevant constituent with respect to potential PBT properties. Therefore, testing the water solubility and log P_{ow} with ppDTBDA **or** poDTBDA DTBDA is required to perform correct bioaccumulation, toxicity and simulation degradation testing.

1.A: Water solubility (OECD 105) (using the column elution method) using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

Considerations on the test method

The OECD 105 guideline recommends for low water soluble substances (< 10 mg/L) the column elution method. Given that the solubility is dependent on the temperature, it is recommended to perform this water solubility test at the same temperature as the simulation study, i.e. 12°C.

1.B Partition Coefficient (1-Octanol/Water): Slow-Stirring Method (OECD 123) or HPLC Method (OECD 117) using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

Considerations on the test method

The OECD guideline recommends for log P_{OW} values of about 7.11 the slow-stirring method (OECD 123) which is accurately for values up to log P_{OW} of 8.2. OECD guideline 117 (HPLC-Method) covers values of log P_{OW} of 0 to 6 and can in exceptional cases cover expanded to log P_{OW} values between 6 and 10. Thus, the appropriateness of the chosen test should be justified accordingly.

Comments from the Registrant(s) on the proposals for amendment

You commented on the PfA suggesting to additionally request tests on water solubility and on log P_{ow} and stated that the timeframe of 18 months for conducting the bioaccumulation and certain pre-tests on solubility and adsorption would not allow to also conduct these OECD tests according to GLP.

Based on your comments on the initial draft decision, the deadline for the bioaccumulation test had already been prolonged from 9 to 18 months to enable pre-tests. It was then presumed that these pre-tests would include a water solubility study according to OECD 105 and a log K_{ow} according to OECD 123 or 117. In your comments on the PfA, you clarified that you did not plan to conduct tests according to GLP within these 9 months. ECHA considers, however, that the additional 9 months would allow conducting the requested tests and therefore this decision gives 9 months for conducting these tests. .

Conclusion

Therefore, based on the substance evaluation and pursuant to Article 46(1) of the REACH Regulation, ECHA concludes that you are required to carry out the following studies using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance subject to this decision:

1.A: Water solubility (OECD 105) (using the column elution method)

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1.B: Partition Coefficient (1-Octanol/Water): Slow-Stirring Method (OECD 123) or HPLC Method (OECD 117)

2. Simulation testing on ultimate degradation in surface water; test method: Aerobic mineralisation in surface water - simulation biodegradation test at 12°C, EU C.25./OECD 309, pelagic test – without additional suspended solids/sediment, using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

The Concern(s) identified and why new information is needed

With regards to the available information on persistence, experimental results are only available for the registered substance and not for the individual constituents. In the registration dossier(s), experimental data on biodegradation is available. One ready biodegradation test (OECD TG 301B) was performed using the registered substance. In the test, 0% degradation (CO_2 evolution) was measured after 28 days. No information regarding simulation testing (within water, soil, or sediment) of the registered substance or its constituents, is available within the registration dossier(s).

Since the pass level was not reached in the biodegradation screening test described above, it can be concluded that the registered substance is not readily biodegradable. Furthermore, the absence of any CO_2 formation during this test suggests that none of the constituents of the UVCB substance could be ultimately degraded under conditions of the ready biodegradation test.

Following an evaluation of the available information, ECHA considers that the registered substance is not readily biodegradable. Furthermore, the available information does not allow the derivation of a degradation half-life ($DegT_{50}$) of the registered substance or its constituents in any environmental compartment. Consequently, the available information does not allow a direct comparison with the P criterion according to Annex XIII. There is a possible risk that the substance meets the persistence (P or vP) criterion of Annex XIII of the REACH Regulation and further data is needed to clarify this concern.

As indicated above, the constituent DTBDA is regarded as the most relevant constituent with respect to potential PBT properties. Therefore, simulation testing with one isomer of the constituent DTBDA ppDTBDA **or** poDTBDA is required to allow a comparison with the Annex XIII criteria of the REACH Regulation.

Determination of environmental compartments exposed to the substance

The determination of the most relevant environmental compartment for simulation testing of DTBDA depends on the use of the registered substance, the physico-chemical properties of DTBDA, and its distribution in different environmental compartments.

The registered substance is used in greases and lubricants. Emission of the substance to the environment can be assumed due to run-off of machines/vehicles to wastewater effluent or direct exposure to soil and water. Due to the low vapour pressure of all constituents of the registered substance (< 0.01 Pa at 25°C) and low Henry's law constant of DTBDA (0.71 Pa m^3/mol at 25°C), volatilisation of DTBDA to air is regarded as unlikely. Therefore, the emission of the substance to air is not relevant. The distribution of DTBDA to air, water, soil and sediment assuming 100% emission to soil and water according to Mackay level III model are shown in Table 1 below. If 100%

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emission to soil is assumed, almost all of DTBDA remains in the soil. Assuming direct emission of DTBDA to water, 64.50% of the substance distributes to sediment whereas 35.50% remains in the water phase.

Table 1. Relative mass distribution (%) of DTBDA according to the Mackay level III (steady state) model of EPISuite v. 4.1 for 100% emission of the constituent to soil, water and sediment.

Compartment	Mass distribution (%) (100% emission to soil)	Mass distribution (%) (100% emission to water)
Air	≤0.01	≤0.01
Water	0.02	35.50
Soil	99.92	≤0.01
Sediment	0.04	64.50

According to the STP (Sewage treatment plant) model, most of DTBDA will be adsorbed to sludge when entering the STP (Table 2). The fraction adsorbed to STP sludge is normally assumed to be disposed of on soil and hence 93.11% of DTBDA is assumed to expose the soil compartment. A relevant fraction of 6.11% will not be removed in the STP and will enter the aquatic environment. Based on the distribution of DTBDA after 100% emission to water (Table 1) it can be assumed that 3.94% of the substance will distribute to sediment and 2.17% remains in the aquatic environment. Only minor amounts of DTBDA (0.78%) is estimated to be degraded in the STP.

Table 2. Relative mass distribution (%) of DTBDA according to the STP model of EPISuite v. 4.1

Removal In Wastewater Treatment:	Mass distribution (%)
Total removal:	93.89
Total biodegradation:	0.78
Total sludge adsorption (potentially deposed of on soil):	93.11
Total to Air:	0
Not removed in the STP, i.e. released to surface water	6.11

Based on the modelling results, water, sediment and the soil are regarded as compartments exposed to DTBDA. Soil will be exposed by direct emission as well as indirectly via the treatment of soil with sewage sludge. Exposure of water will occur by direct emission and via STP; sediment will be indirectly exposed via the water phase. Therefore, surface water, soil and sediment are regarded as relevant compartments for simulation testing of DTBDA.

Determination of the testing strategy

The constituent DTBDA has a high adsorption potential (log K_{oc} = 4.64) to soil/sediment and a low water solubility (S_w = 0.014 mg/L). Thus, DTBDA will adsorb to solid and suspended matter and will most likely show a high non-extractable residue (NER) formation. Interpretation of NER is, however, not straightforward and still a topic of scientific debate, e.g. because the unknown composition of NER with respect to the parent and formed metabolites as well as the irreversibility of the binding to soil, sediment or organic matter. The NER should ideally be differentiated in remobilisable and irreversibly bound fractions. While the irreversibly bound part (e.g. biogenically bound) can be assessed as a potential removal pathway, the remobilisable fraction (heavily

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sorbed, physical inclusion) pose a potential emission source for the environment. Moreover, NER formation in a soil simulation test, sediment simulation test and surface water simulation test with the addition of suspended solids can complicate a reliable determination of the degradation half-life of the parent compound. In surface water simulation tests without artificially added suspended matter (pelagic version), the SPM concentration and subsequent NER formation is low, which minimises the above mentioned interpretation problems related to the likely NER formation. Therefore, preference is given to a simulation test of DTBDA in surface water without the addition of suspended solids, if considered technically feasible due to the low water solubility of DTBDA (S_w = 0.014 mg/L).

Considerations on the test method

The OECD 309 simulation test should be performed using ^{14}C-radiolabelled ppDTBDA **or** poDTBDA. According to OECD 309, ^{14}C-radiolabelling of the most stable part of the molecule ensures the determination of the total mineralisation. The radiolabel should be located in the most stable part of the molecule, i.e. the aromatic ring in case of ppDTBDA and poDTBDA . ppDTBDA and poDTBDA contain two aromatic rings linked by a nitrogen atom. For substances containing more than one aromatic ring it is recommend that each ring should preferably be ^{14}C-labelled (OECD 309).

The test setup shall make it possible to perform a mass balance and the identification of transformation products relevant for PBT assessment. OECD 309 shall employ a SPM concentration of naturally occurring surface water SPM between 10 and 20 mg/L. Furthermore, when reporting NER in your test you should explain and scientifically justify the extraction procedure and solvent used obtaining a quantitative measure of NER. During the test duration, transformation products of ppDTBDA **or** poDTBDA should be analysed by means of the ^{14}C-radiolabel.

Studying the degradation of ppDTBDA **or** poDTBDA in surface water is expected to be technically feasible because the ^{14}C-radiolabel allows testing the degradation of the substance below its water solubility limit of 0.014 mg/L. With regard to OECD 309, the used test concentration of ppDTBDA **or** poDTBDA should ensure that the biodegradation follows first order kinetics.

At present, a test temperature of 12°C is considered by authorities as the mean temperature of European surface waters and is required by the ECHA Member State Committee to be used as the testing temperature for new simulation degradation tests. Therefore, in order to simulate as much as possible the real environmental conditions in the EU, but avoiding to perform the test at multiple temperatures, it is deemed appropriate to conduct this surface water simulation test at 12°C.

The test shall be performed without the addition of coarse particles (i.e. a pelagic test type) because adsorption to solid carbon will reduce the bioavailability of the test item and thus diminish the reliability of the test. According to the test on ready biodegradation, the UVCB substance may degrade slowly (0% CO2 after 28 days) due to long lag time of degrading microorganisms in the test. Regarding the OECD 309 test guideline, prolonged incubation time may be required in order to achieve a sufficient degradation of such recalcitrant substances in a surface water simulation test. To adequately determine the degradation of the isomer ppDTBDA **or** poDTBDA, the incubation period of the surface water simulation test could be extended from 60 days to a maximum of 90 days. The batch test can be extended to a maximum of 90 days

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without starting a semi-continuous procedure, if degradation of ppDTBDA **or** poDTBDA (monitored by $^{14}CO_2$ evolution and the occurrence of transformation products) can be detected within the first 60 days. If no degradation of ppDTBDA **or** poDTBDA can be detected within the first 60 days of incubation, the batch procedure should be changed into a semi-continuous procedure for the remaining 30 days of incubation.

Consideration of Registrants' comments

In your comments on the initial draft decision you agreed to conduct simulation degradation testing with the isomers of the most relevant constituent. However, you also stated that, if a simulation test on ultimate degradation in surface water is technically feasible, you disagree that the surface water should not be amended with suspended sediments. You stated that according to OECD Guideline 309, 0.01 to 1 g/l dry weight suspended solids or sediment can be present in the test system and you disagreed to deviate from this concentration range. The appropriate SPM concentration would be elaborated during the test once the test is being conducted. Furthermore, the presence of suspended solids in simulation tests with surface water is not excluded according to Chapter R.11 (PBT Assessment) of ECHA's Guidance on information requirements and chemical safety assessment (June 2017).

ECHA does not agree that the test on ultimate degradation in surface water, if technically feasible, should be performed with suspended sediment. DTBDA is deemed to form NER because of the strong adsorption potential of DTBDA to sediment (log K_{oc} =4.64). Shrestha et al. (2016) indicated that in a test on ultimate degradation in surface water with suspended sediment also NER-formation occurs. NER formation in a soil simulation test, sediment simulation test and surface water simulation test with the addition of suspended solids can complicate a reliable determination of the degradation half-life of the parent compound. In surface water simulation tests without artificially added suspended matter (pelagic version), the NER formation is low, which minimises the above mentioned interpretation problems related to the likely NER formation. Therefore a test on ultimate degradation in surface water shall be performed as pelagic version without the addition of suspended sediment.

Deadline to submit the requested Information

In the draft decision communicated to you, the timeline indicated to provide the requested simulation degradation tests was 27 months from the date of adoption of the decision. In your comments on the draft decision, you requested an extension of the timeline to 48 months. You sought to justify this request with a statement from the test laboratory indicating that 12 months are needed for the radiolabelled synthesis and certification. Furthermore, based on the current workload and capacity of the test facility, a further 24 months are needed if only one study must be performed, and additionally 12 months if the second simulation degradation test must be performed.

Concerning the additional 12 months you proposed for the radiolabelled synthesis and certification, ECHA notes that only one laboratory was contacted to perform the radiolabelled synthesis and certification. This laboratory states that 12 months are needed to perform radiolabelled synthesis and certification.

Concerning the laboratory capacity, ECHA notes that you have contacted only one laboratory to perform the originally requested OECD 309 and OECD 308 studies. This laboratory states that 36 months are needed to perform both tests. It appears that you have not thoroughly checked if alternative laboratories might have the capacities to

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conduct the requested simulation testing study. Thus, ECHA cannot follow the argumentation that there is a lack of laboratory capacity.

Proposals for amendment by other MSCAs and ECHA

PfAs from four MSCAs were submitted regarding the persistence testing strategy. The conditional OECD 308 test in sediment was removed following the PfAs.

Comments from the Registrant(s) on the proposals for amendment

In your comments on PfAs by the other MSCAs and ECHA, you agreed to the PfAs of two MSCAs to conduct a simulation testing on degradation in one compartment as worst case and to extrapolate to the other compartments. The scenario for conducting a second simulation test (OECD 308) which was originally requested in the draft decision was removed from the testing strategy for this decision.

You again stated that the presence of suspended solids in simulation tests with surface water is not excluded according to Guidance on Information Requirements and Chemical Safety Assessment Chapter, R.11: PBT/vPvB assessment Version 3.0 June 2017. ECHA does not agree for reasons stated above.

You again stated that with the given deadline, it is not possible to provide the study results or the final study reports by the deadline. ECHA refers to its above observations on this matter.

Conclusion

Therefore, based on the substance evaluation and pursuant to Article 46(1) of the REACH Regulation, ECHA concludes that you are required to carry out the following study using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance subject to this decision:

2. Simulation testing on ultimate degradation in surface water; test method: Aerobic mineralisation in surface water - simulation biodegradation test at 12°C, EU C.25./OECD 309, pelagic test – without additional suspended solids/sediment.

If the simulation study results in the substance being not P/vP in the tested compartment and these results are sufficient to conclude on persistence in other environmental compartments, no additional simulation tests will be needed. If a concern on the persistence in some of the compartments remains, the evaluating MSCA may consider whether further simulation testing needs to be requested in future SEV decisions.

3. Bioaccumulation in aquatic species; test method: Bioaccumulation in fish: aqueous and dietary exposure, OECD 305, aqueous exposure using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

This request is dependent on the outcome of the simulation test in water (OECD 309) above. If the outcome of the test requested under 2 allows to conclude that ppDTBDA **or** poDTBDA is persistent (P) or very persistent (vP) according to Annex XIII of the REACH Regulation, an OECD 305 test is required.

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The Concern(s) Identified and why new information is needed

With regards to the available information on bioaccumulation, experimental results are not available for the registered substance or the individual constituents. The registered substance and its main constituents have a log P_{ow} >4.5 and thus exceed the screening criterion for bioaccumulation (log P_{ow} >4.5) as specified in Chapter R.11 (PBT Assessment) of ECHA's Guidance on information requirements and chemical safety assessment (June 2017). Therefore, the registered substance must be considered as potentially B/vB.

Based upon the available data on bioaccumulation a weight-of-evidence approach conducted by the evaluating MSCA balancing physico-chemical properties and different QSAR estimations of the identified constituents as well as one experimental BCF study provided by you with the read-across candidate 4-nonyl-N-phenylaniline (CAS 27177-41-9) suggest a high bioaccumulation potential of the registered substance. The reasons are as follows:

i) According to Chapter R.11 of ECHA's Guidance on information requirements and chemical safety assessment (June 2017), a molecular weight above 700 g/mol plus an average molecular diameter greater than >17 Å is an indicator that the substance's BCF is below 5000 L/kg. All relevant constituents of the registered substance have a molecular weight below 700 g/mol (between 225.35 and 505.88 g/mol). Furthermore, you calculated the average molecular diameter of the different constituents to be below 17 Å (between 14.09 Å and 13.38 Å), using CATALOGIC. Therefore, all constituents are considered sufficiently bioavailable and it cannot be excluded that the registered substance is vB.

ii) QSAR estimations provided by you to estimate BCF values of relevant constituents using the BCF/BAF tool of EPISuite and the BCF baseline model of Catalogic revealed regression based BCF values in the range between 1250 and 12500 L/kg w.w. (Appendix 4, Table 1). Also the BCF values assessed for lower trophic levels applying the Arnot-Gobas model and incorporating the mitigating factor biotransformation lie between 17 and 6761 L/kg w.w. As among all constituents Group A has the highest estimated Arnot-Gobas BCF values (Monotertoctyldiphenylamine: 2667 L/kg and DTBDA: 6761 L/kg w.w.), this group is considered to have the highest potential for bioaccumulation and therefore to represent the most relevant constituents of the UVCB regarding PBT properties. Information based on QSAR calculations shall be used only as part of an overall weight-of-evidence approach beside other available information from testing and non-testing data. Hence a decisive conclusion whether any of the constituents of the registered substance meets the vB/B criterion cannot be drawn solely based on this screening information.

iii) A thorough evaluation of the experimental bioaccumulation study with 4-nonyl-N-phenylaniline (CAS 27177-41-9) according to the Substances Control Law of Japan (MITI, 1998), which was proposed by you as a read-across study for bioaccumulation, revealed technical and statistical deficiencies. It could not be concluded from the measurements that the bioconcentration had reached a steady state. According to OECD 305, a steady-state is reached in the plot of test substance in fish (C_f) against time when the curve becomes parallel to the time axis and three successive analyses of C_f made on samples taken at intervals of at least two days are within ±20% of each other, and there are no significant increases among the three sampling periods. As in the provided test no plateau of uptake phase was reached because the fish concentrations of the last three

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measurements during uptake phase varied more than 20% of each other, the steady state BCF cannot be applied and a kinetic BCF has to be calculated. Calculation of kinetic lipid normalized BCF of 4-nonyl-N-phenylaniline using the experimental data of the test and a Box-Cox transformation for curve fitting (proposed as optimal statistical procedure for curve fitting in the recently revised Guidance Document for the OECD 305, 2016) yields in a $BCF_{lip+kin}$ of 2190 L/Kg, exceeding the threshold for bioaccumulation.

According to REACH legal text, particularly Annex XI, 1.5 and the 'Read-across framework (RAAF)'[5] recently published by ECHA, substance similarity may be based on three criteria:

(i) a common functional group;
(ii) common precursors and/or the likelihood of common breakdown products via physical and biological processes, which result in structurally similar chemicals; or
(iii) a constant pattern in the changing of the potency of the properties.

All three points are only met for one monoalkylated constituent of the registered substance, namely Monotertoctyldiphenylamine, as this substance differs only in the chain branching as well as the chain length and has similar physico-chemical properties compared to 4-nonyl-N-phenylaniline. Hence, the read-across from 4-nonyl-N-phenylaniline is justified for this constituent of the registered substance indicating that Monotertoctyldiphenylamine likely meet the B criterion (BCF > 2000 L/kg). Therefore, according to the read-across, it cannot be excluded that Monotertoctyldiphenylamine also fulfils the B/vB criterion according to Annex XIII of the REACH regulation.

However, Monotertoctyldiphenylamine is not the most relevant candidate of the the registered substance constituents regarding the potential for bioaccumulation. Based on the bioaccumulation potential according to estimated BCF values for the constituents of the registered substance, DTBDA (BCF [Arnot-Gobas]= 6761 L/kg) is regarded as the most relevant candidate for bioaccumulation.

The suggested read-across bioaccumulation study using 4-nonyl-N-phenylaniline has fundamental deficiencies, as the read-across is only justified for one constituent (Monotertoctyldiphenylamine), within the study a steady state concentration in fish was not reached, and the statistical evaluation provided by you is not appropriate. Hence, the provided read-across study does not allow a decisive conclusion regarding the B or even vB status. There is no further information about bioaccumulation of the registered substance in the registration dossier.

Following an evaluation of the available information, ECHA considers that the registered substance and its main constituents have a high potential for aquatic bioaccumulation. However, the available information is not sufficient to enable an unequivocal conclusion regarding their bioaccumulation potential. Consequently, one or more constituents of the registered substance may meet the bioaccumulation (B or vB) criterion of Annex XIII of the REACH Regulation and further data is needed to clarify this concern. This necessary information should be generated according to the above-mentioned testing strategy, by assessing ppDTBDA **or** poDTBDA in a bioaccumulation study according to OECD 305 to

[5] European Chemicals Agency (2015) Read-Across Assessment Framework (RAAF).

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ensure that the information generated is adequate for comparison with the Annex XIII criteria of REACH.

Considerations on the test method

In general, aqueous exposure should be used in OECD 305 test because decisive BCF trigger values for B and vB exist under REACH Annex XIII in contrast to the biomagnification factor (BMF). Unlike BCF values, the BMF values are not directly comparable to REACH Annex XIII B/vB criteria. Thus, a BCF derived from aquatic exposure test allows to decide if a substance is B/vB because BCF trigger values for B/vB are defined under REACH Annex XIII in contrast to the biomagnification factor (BMF).

OECD TG 305 states "The aqueous exposure test is most appropriately applied to stable organic chemicals with log P_{OW} values between 1.5 and 6.0 (13)...". However, OECD 305 specifications continue with "[...] but may still be applied to strongly hydrophobic substances (having log P_{OW} > 6.0), if a stable and fully dissolved concentration of the test substance in water can be demonstrated." Furthermore, OECD TG 305 states that there should be a preference for aqueous exposure bioaccumulation (i.e. bioconcentration) studies to be run when "technically feasible" (see paragraph 10 of the TG). Thus the requirement of an OECD 305 test using aqueous exposure is in line with the current scientific concept albeit the log P_{OW} is > 6 and the bioaccumulation test is requested to be performed with aqueous exposure.

A water solubility below ~0.01 mg/L marks the limit below which testing via aqueous exposure may become increasingly difficult. The test compound DTBDA has a calculated water solubility of 0.014 mg/L. Thus the water solubility is considered sufficient to conduct the bioaccumulation test with aqueous exposure. A flow-through system is recommended, and solvents can be applied in accordance with the test guideline. The OECD guidance document to OECD 305 describes more advanced dosing systems for highly lipophilic substances, e.g. SPME, that may warrant a stable substance concentration in water and should be considered for the test with ppDTBDA **or** poDTBDA.

Therefore, the bioaccumulation test is requested to be performed with aqueous exposure. Only if it is justified that the test is documented to be technically unfeasible to conduct with aqueous exposure with reasonable efforts, the test can be conducted with dietary exposure.

Radiolabeled test substance shall be used along with parent substance analysis to allow an assessment of the relevant contribution of the metabolite to any observed accumulation. The organic carbon content of the test water (e.g. from fish excreta and food residues) should be kept as low as possible, and efforts shall be made to establish the truly dissolved concentration, for example by taking measurements of particulate and dissolved organic carbon concentrations at appropriate time points and using an appropriate technique to enable the estimation of the bioavailable fraction if feasible (e.g. solid-phase micro-extraction). Excessive fish growth and lipid increases should also be avoided since these might influence the results. The results should in any case be corrected for growth and normalized to 5% lipid content.

Alternative approaches and proportionality of the request

As stated within Chapter R.11 of the above mentioned Guidance, when deciding on the persistence, bioaccumulation or toxicity information required to reach an unequivocal

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conclusion, vertebrate animal testing must be avoided whenever possible. Therefore, when further information for several properties is required, the assessment should normally clarify the potential for persistence first. When it is clear that the P criterion is fulfilled, a stepwise approach is followed to clarify whether the B criterion is fulfilled.

Therefore, the information requested within the present decision is requested sequentially and first focusses on the need to clarify the P properties of the registered substance, followed by clarification of the B properties of the registered substance, if needed. Consequently, an OECD 305 test is only required if, on the basis of the simulation test requested under 2, it is concluded that ppDTBDA **or** poDTBDA is persistent (P) or very persistent (vP) according to Annex XIII of the REACH Regulation.

Without the bioaccumulation fish test according to OECD 305, no definitive conclusion can be made regarding the PBT properties of the registered substance. The request for bioaccumulation testing is suitable and necessary to obtain information that will clarify whether the registered substance is bioaccumulative (B) or very bioaccumulative (vB) according to Annex XIII of the REACH Regulation. More explicitly, there is no equally suitable alternative way available of obtaining this information. ECHA notes that there is no experimental study available at this stage that will generate the necessary information and which does not require testing on vertebrate animals. Consequently, the bioaccumulation study according to OECD 305 with fish using ppDTBDA **or** poDTBDA as test substance is required to investigate whether the B/vB criterion according to REACH Annex XIII is met in line with the information requests on persistence and toxicity.

Consideration of Registrants' comments

In your comments on the draft decision, you agreed to conduct a bioaccumulation study if the substance is persistent or very persistent according to REACH Annex XIII.

Deadline to submit the requested Information

In the draft decision communicated to you, the time indicated to provide the requested bioaccumulation study was 9 months. In your comments on the draft decision, you requested an extension of the timeline to 18 months. You sought to justify this request with a statement from the test laboratory indicating that 18 months are needed due to laboratory capacity and the difficult properties of the test substance. More specifically, the test laboratory states that DTBDA has difficult properties and no experimental data on solubility and adsorption in aquatic test media are available. A set of pre-tests must be performed and the saturation limit in the test medium has to be determined before starting the main bioaccumulation test.

Concerning the laboratory capacity, ECHA notes that only one laboratory was contacted by you to perform the requested OECD 305 study. This laboratory states that 18 months are needed to perform the test. No further laboratories were questioned by you regarding the conduction of the requested OECD 305 study. It appears that you have not thoroughly checked if alternative laboratories might have the capacities to conduct the requested OECD 305 test. Thus, ECHA cannot follow the argumentation that there is a lack of laboratory capacity.

Concerning the difficult properties of the test substance, ECHA agrees that no experimental data on solubility and adsorption in aquatic test media are available for DTBDA. However, according to the OECD 305 test guideline, information on the water solubility of test substance should be known before carrying out any of the bioaccumulation tests. However, as indicated within section 1 above, requests to

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determine both water solubility (OECD 105) and log Kow (OECD 123 or 117) are included within this Decision (information requirements 1A and 1B).

Therefore, ECHA has not granted the request to extend the deadline for conducting the OECD 305 test.

Conclusion

Therefore, based on the substance evaluation and pursuant to Article 46(1) of the REACH Regulation and depending on the outcome of the persistence requirements, ECHA concludes that you are required to carry out the following study using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance subject to this decision:

Bioaccumulation in aquatic species; test method: Bioaccumulation in fish: aqueous exposure, OECD 305.

4 Toxicity testing

This request is dependent on the outcome of the persistency testing (OECD 309) and the bioaccumulation testing (OECD 305). If the outcome of the tests requested under 2 and 3 allows concluding that ppDTBDA **or** poDTBDA is either I) persistent (P) and bioaccumulative (B), II) very persistent (vP) and bioaccumulative (B) or III) persistent (P) and very bioaccumulative (vB) according to Annex XIII of the REACH Regulation, toxicity testing (OECD 211, OECD 201 and OECD 210) is required.

If the outcome of the tests requested under 2 and 3 allows to conclude that ppDTBDA **or** poDTBDA is either I) very persistent (vP) and very bioaccumulative (vB) or II) not persistent (P) or not bioaccumulative (B), toxicity testing (OECD 211, OECD 201 and OECD 210) can be waived.

The Concern(s) identified and why new information is needed

In the registration dossier(s), data regarding short-term and long-term toxicity of the registered substance on aquatic organisms are available. No reliable information on the toxicity of the constituents on aquatic organisms is available. The available data on aquatic toxicity of the registered substance does not allow the derivation of a NOEC or EC_{10} for the single constituents. Furthermore, the constituents are poorly soluble in water and sufficient information on analytical monitoring is not available. OECD (2002), Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures states that "where poorly soluble components in the multi-component substances are of concern, the WAF method is not adequate to determine the toxicity of such multi-component substances". The most relevant constituent DTBDA (with respect to potential PBT properties) is poorly soluble, therefore, the WAF method is not adequate to allow a comparison with the Annex XIII criteria of the REACH regulation.

A testing proposal for an OECD 443 test on the registered substance is currently being evaluated by ECHA. Therefore, a final assessment on mammalian toxicity of the registered substance is not yet possible. However, it would not be possible to identify to which extent the individual constituent(s) cause any effects observed in the proposed OECD 443 test performed with the whole UVCB substance.

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The available information is insufficient to allow an assessment of the ecotoxicological effects of the individual constituents. Consequently, there is a possible risk that the individual constituents meet the toxicity (T) criterion and further data is needed to clarify this concern. This necessary information should be generated according to the above-mentioned testing strategy, by assessing ppDTBDA **or** poDTBDA in long-term toxicity studies to ensure that the information generated is adequate for comparison with the Annex XIII criteria of REACH.

Based on the available toxicity data, it cannot be concluded that one taxonomic group is significantly more sensitive towards ppDTBDA **or** poDTBDA than the others. Due to animal welfare concerns, the long-term toxicity tests shall be conducted sequentially in order to avoid unnecessary vertebrate animal testing; tests under 4.A (OECD 211) and 4.B (OECD 201) should be conducted first. In case the OECD 211 and 201 do not allow concluding that ppDTBDA **or** poDTBDA fulfils the T-criterion according to Annex XIII of the REACH Regulation, the OECD 210 test is required.

4.A: Long-term toxicity testing on aquatic invertebrates; test method: *Daphnia magna* reproduction test, EU C.20./OECD 211 using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

Information from three short-term studies on toxicity to aquatic invertebrates are available in the registration dossier(s). A key study (OECD 202) was conducted with the registered substance and the relevant endpoint mobility is based on loading rates. You have justified this approach on the basis that the analytically measured concentrations are neither correlated with the loading rates nor the immobility of the daphnids. However, the measured concentrations were below LOQ in the treatment with the lowest test concentration and were well below the loading rates in all other treatments. Since no relationship of the measured concentrations and the endpoint immobility can be established, and the registered substance is poorly soluble in water, ECHA considers that this test does not allow a conclusion on the toxicity of the single constituents of the registered substance.

In a supporting OECD 202 study ([redacted]. 1998) a 24h limit-test was conducted on the registered substance. After 24h, 100% mortality was observed, however, no analytical monitoring was performed and the EC_{100} is stated as <100 mg/L. Chapter R.7b of ECHAs Guidance on information requirements and chemical safety assessment (February 2016) states 'Where a test result is reported as a less than (<) value this cannot be used.' Therefore, based on this study, no conclusion on the toxicity of the registered substance or the single constituents can be drawn.

In a second supporting OECD 202 study ([redacted]. 2004b) a limit test was conducted on a read-across UVCB substance (EC [redacted]) containing the constituent [redacted]. No toxic effect on Daphnia magna at a loading rate of 100 mg/L was reported. However, the analytical monitoring shows measured concentrations below the LOQ (< 0.0024 mg/L). Therefore no conclusion can be drawn on the read-across constituent [redacted].

Information from one long-term study on toxicity to aquatic invertebrates is available in the registration dossier(s). This key study (OECD 211) was conducted with the registered substance and reported an EL_{10} of 1.69 mg/L and a NOELR of <0.625 mg/L based on the most sensitive endpoint (reproduction). According to you, no analytical monitoring was conducted, since in the acute study with Daphnia magna ([redacted].

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2004a) there was no relationship among measured concentrations and observed effects. However, most constituents of the registered substance are poorly water soluble. The provided acute studies show a large deviance between measured concentrations and loading rates. From the results of the test it can be concluded that single constituents of the registered substance are toxic to aquatic invertebrates, but not at which concentrations.

QSAR estimations (see Annex 4, Table 1) on the toxicity of relevant para substituted constituents of the registered substance to aquatic organisms also indicate that some of the constituents, including DTBDA, may have NOEC values below the T cut-off value of 0.01 mg/L and thus may be regarded as potentially T. Consequently, individual constituents, including DTBDA, may meet the toxicity (T) criterion and further data is needed to clarify this concern.

Therefore, a long-term toxicity test on aquatic invertebrates with ppDTBDA **or** poDTBDA is required to conclude on the T criteria.

Considerations on the test method

Due to the low solubility of the substance in water, the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (OECD 2016) and ECHA Guidance, Chapter R7b (2016) summarising aquatic toxicity testing of difficult substances shall be consulted by you for choosing the design of the requested long-term ecotoxicity tests and for calculation as well as expression of the results of the tests.

4.B: Growth inhibition study aquatic plants; test method: Algae, growth inhibition test, EU C.3./OECD 201 using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

Information from two studies on toxicity to algae and aquatic plants are available in the registration dossier(s). A key study (OECD 201) was conducted with the registered substance. No information is provided regarding analytical monitoring or whether the validity criteria were met. The determined NOEC (based on water accommodated fractions) is 10 – 100 mg/L, however, no explanation is provided as to why a concentration range is given. As shown in acute studies with Daphnia magna, there is a large deviance between measured concentrations and loading rates. Therefore, no conclusion on the toxicity of the single constituents of the registered substance can be drawn.

A second supporting study (OECD 201) was conducted with a read-across UVCB containing mainly [redacted] ([redacted]%) and [redacted] ([redacted]%). As in the key study, no information is provided regarding analytical monitoring or whether the validity criteria were met. Consequently, the available information is insufficient to allow an assessment of the ecotoxicological effects of the individual constituents.

QSAR estimations (see Annex 4, Table 1) on the toxicity of relevant para substituted constituents of the registered substance to aquatic organisms indicate that some of the constituents are toxic and might be regarded as potentially T. Consequently, there is a possible risk that the individual constituents meet the toxicity (T) criterion and further data is needed to clarify this concern.

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Therefore, a growth inhibition study with aquatic plants with ppDTBDA **or** poDTBDA is required to conclude on the T criteria.

Considerations on the test method

Due to the low solubility of the substance in water the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, (OECD 2002) and ECHA Guidance, Chapter R7b (2016), summarising aquatic toxicity testing of difficult substances shall be consulted by you for choosing the design of the requested long-term ecotoxicity tests and for calculation as well as expression of the results of the tests.

4.C: Long-term toxicity testing on fish; test method: Fish, early-life stage (FELS) toxicity test, OECD 210 using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance

This request is dependent on the outcome of the long-term toxicity testing on aquatic invertebrates (OECD 211) (4.A) and of the results of the growth inhibition study on aquatic plants (OECD 201) (4.B) above. In case the OECD 211 and OECD 201 do not allow concluding that ppDTBDA **or** poDTBDA fulfils the T-criteria according to Annex XIII of the REACH Regulation, long-term toxicity testing on fish (OECD 210) is required.

Information from one short-term study on toxicity to fish is available in the registration dossier(s). A key study (OECD 203) was conducted with the registered substance. The maximum vehicle concentration in the test (950 mg/L Dimethylformamide and 0.8 mg/L alkylphenol-polyglykol-ether) is above the maximum vehicle concentration specified in OECD 203 test guideline (100 mg/L). Furthermore, the endpoints are based on nominal concentrations. Despite the high vehicle concentration, the measured test concentrations deviate strongly from the nominal test concentrations.

As stated in Chapter R.7b (Table R.7.8—2) of ECHAs Guidance on information requirements and chemical safety assessment (February 2016), very high vehicle concentrations are very likely to influence the toxicity of the test substance. For UVCB substances, vehicles should generally be avoided, as a preferential solution can result. Furthermore water-accommodated fractions (WAF) have to be used for UVCB substances. In this study a single stock WAF instead of individually prepared WAFs was used, which is not appropriate (Table R.7.8—2 of the abovementioned Guidance). For these reasons, ECHA considers the study to be invalid and cannot be considered for the toxicity assessment. Consequently, no reliable information on the toxicity of the registered substance on fish is currently available.

In addition, QSAR estimations (see Annex 4, table 1) on the toxicity of relevant para substituted constituents of the registered substance to aquatic organisms indicate that some of the constituents are toxic and might be regarded as potentially T. Consequently, there is a possible risk that the individual constituents meet the toxicity (T) criterion and further data is needed to clarify this concern. ECHA considers the study to be invalid with respect to PBT assessment. Therefore, a long-term toxicity test on fish with ppDTBDA **or** poDTBDA is required to conclude on the T criteria.

Considerations on the test method

Due to the low solubility of the substance in water the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, (OECD 2002) and ECHA

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Guidance, Chapter R7b (2016), summarising aquatic toxicity testing of difficult substances shall be consulted by you for choosing the design of the requested long-term ecotoxicity tests and for calculation as well as expression of the results of the tests.

Alternative approaches and proportionality of the request

As stated within Chapter R.11 of the abovementioned Guidance, when deciding on the persistence, bioaccumulation or toxicity information required to reach an unequivocal conclusion, vertebrate animal testing must be avoided whenever possible. Therefore, when further information for several properties is required, the assessment should normally clarify the potential for persistence first. When it is clear that the P criterion is fulfilled, a stepwise approach is followed to clarify whether the B criterion is fulfilled, followed by clarification of the T criterion.

Therefore, the information requested within the present decision is requested sequentially and first focusses on the need to clarify the P and B properties of the registered substance, followed by clarification of the T properties of the registered substance, if needed. Consequently, long-term aquatic toxicity tests are only required if, on the basis of the tests requested under 2 and 3, it is concluded that ppDTBDA **or** poDTBDA is either I) persistent (P) and bioaccumulative (B), II) very persistent (vP) and bioaccumulative (B) or III) persistent (P) and very bioaccumulative (vB) according to Annex XIII of the REACH Regulation.

Furthermore, the long-term toxicity tests shall be conducted sequentially in order to avoid unnecessary vertebrate animal testing; tests under 4.A (OECD 211) and 4.B (OECD 201) are to be conducted first. Only in case the OECD 211 and 201 do not allow concluding that ppDTBDA **or** poDTBDA fulfils the T-criterion according to Annex XIII of the REACH Regulation, the OECD 210 test is required.

Long-term studies using ppDTBDA **or** poDTBDA on aquatic organisms are necessary to investigate whether the T-criterion is met in line with the information requests on bioaccumulation and persistence. The assessment of the T criteria as conducted by you is not appropriate, as the provided studies on which the assessment is based are not suitable to conclude on the T criteria according to Annex XIII. Furthermore, available tests on short- and long-term toxicity on aquatic organisms using the registered substance do not allow a conclusion which organism (aquatic invertebrates, algae or fish) is the most sensitive one. Therefore, aquatic long-term toxicity tests according to OECD 201, OECD 211 and OECD 210 are needed to conclude if ppDTBDA **or** poDTBDA meets the Annex XIII criteria for toxicity (T). The long-term toxicity tests according to OECD 201, OECD 211 and OECD 210 are not required if the requested bioaccumulation testing shows that this isomer does not meet the Annex XIII criteria for B or vB (in which case it can be concluded that the constituent is not PBT and not vPvB) or does meet the Annex XIII criteria for vP and vB (in which case it can be concluded that the isomer is vPvB).

Consideration of Registrants' comments

In your comments on the draft decision, you agreed to the sequential toxicity testing strategy with the isomers of the most relevant constituent and to start the tests 4.A and 4.B if the previous tests allow to conclude that the substance is P/B, vP/B or P/vB according to Annex XIII of the REACH Regulation.

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In addition, you stated that, in case the pre-test with fish for the bioaccumulation study revealed that the substance fulfils the T criterion according to Annex XIII of the REACH Regulation, no further toxicity testing is needed. If no fish toxicity is observed in the bioaccumulation study and the corresponding pre-test and if the results of the studies with algae and Daphnia reveal that the constituent does not fulfil the T-criterion according to Annex XIII of the REACH Regulation, the need to perform a chronic fish toxicity study according to OECD 210 will have to be re-evaluated and should be avoided due to animal welfare.

ECHA does not agree with your statement because test conditions of a pre-test are not comparable to those of an OECD 210 test. This is because in general, the OECD 305 test is not designed to assess the toxicity of a substance. In pre-tests with fish on bioaccumulation no effect on the fish are examined and no dose-response curve could be derived. Therefore, pre-test with fish for the bioaccumulation study cannot be used to conclude that no further toxicity testing is necessary. Furthermore, the absence of toxicity in the i) pre-test with fish of the bioaccumulation study, ii) the OECD algae study and iii) OECD daphnia study cannot be used to conclude that the requested FELS test can be waived. If the results of the studies with algae and Daphnia reveal that the constituent does not fulfil the T-criterion according to Annex XIII of the REACH Regulation, a chronic fish toxicity study according to OECD 210 will have to be performed.

Furthermore, you stated that there is a pending testing proposal for the registered substance for reproductive toxicity study in rats. According to the draft Implementing Decision by the European Commission of December 2016, this process has to be revisited and replaced with a testing proposal for a study according to OECD 443. In case the results of this test are available before the aquatic toxicity tests start and indicate that the registered substance fulfils the T-criterion according to Annex XIII of the REACH Regulation, the necessity to perform aquatic toxicity tests has to be re-evaluated.

ECHA notes that the proposed OECD 443 test may be performed with the registered substance and therefore could not be used to conclude on the toxicity of individual constituents, which is the approach defined for the PBT assessment. Since the registered substance is a UVCB containing different constituents at varying concentrations, the physico-chemical properties and toxicity of the constituents are expected to differ. Consequently, it would not be possible to identify to which extent the individual constituent(s) cause any effects observed in the proposed OECD 443 test performed with the whole UVCB substance.

Deadline to submit the requested toxicity text information (requirements 4A, 4B and 4C)

In the draft decision communicated to you, the time indicated to provide the requested algae and Daphnia reproduction tests was 9 months and the time indicated to provide the requested FELS test was 12 months. In your comments on the draft decision, you requested an extension of the timelines to 18 months for the algae and Daphnia reproduction tests, and 24 months for the FELS test. You sought to justify this request with a statement from the test laboratory indicating that the additional time is needed due to laboratory capacity and the difficult properties of the test substance. More specifically, the test laboratory states that DTBDA has difficult properties for aquatic testing and extensive preliminary tests will be required to compensate for these

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properties and obtain stable exposure concentrations.

Concerning the laboratory capacity, ECHA notes that you contacted only one laboratory to perform the requested OECD 201, 211 and 210 studies. This laboratory states that 18 months are needed to perform the algae and Daphnia reproduction tests and 24 month for the FELS test. It appears that you have not thoroughly checked if alternative laboratories might have the capacities to conduct the requested OECD 201,211 and 210 studies. Thus, ECHA cannot follow the argumentation that there is a lack of laboratory capacities.

ECHA agrees to your statement that DTBDA has difficult properties such as low water solubility which might challenge the aquatic testing. According to the OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (OECD 2002) preliminary tests regarding maximum dissolved concentration, application method and used solvents are necessary prior to conduct toxicity testing with substance showing low water solubility.

Therefore, ECHA has partially granted the request and set the deadline to 18 months for the conduction of algae and Daphnia reproduction tests.

Conclusion

Therefore, pursuant to Article 46(1) of the REACH Regulation, you are required to carry out the following studies using the isomer ppDTBDA or poDTBDA of the constituent DTBDA of the registered substance subject to this decision:

4.A Long-term toxicity testing on aquatic invertebrates; test method: *Daphnia magna* reproduction test, EU C.20./OECD 211. The low water solubility shall be taken into account.
and

4.B Growth inhibition study aquatic plants; test method: Algae, growth inhibition test, EU C.3./OECD 201. The low water solubility shall be taken into account.

In case the result of the test under request 4.A and 4.B does not allow concluding that the registered substance is toxic (T) according to Annex XIII of the REACH Regulation the following test is required:

4.C Long-term toxicity testing on fish; test method: Fish, early life-stage (FELS) toxicity test, OECD 210. The low water solubility shall be taken into account.

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Appendix 2: Procedural history

On the basis of an opinion of the ECHA Member State Committee and due to initial grounds for concern relating to PBT/vPvB properties, exposure of environment as well as wide dispersive use Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene CAS No 68411-46-1 (EC No 270-128-1) was included in the Community rolling action plan (CoRAP) for substance evaluation to be evaluated in 2016. The updated CoRAP was published on the ECHA website on 22 March 2016. The Competent Authority of Germany (hereafter called the evaluating MSCA) was appointed to carry out the evaluation.

Pursuant to Article 45(4) of the REACH Regulation the evaluating MSCA carried out the evaluation of the above substance based on the information in your registration(s) and other relevant and available information.

The evaluating MSCA considered that further information was required to clarify the abovementioned concerns. Therefore, it prepared a draft decision pursuant to Article 46(1) of the REACH Regulation to request further information. It submitted the draft decision to ECHA on 20 March 2017.

The decision making followed the procedure of Articles 50 and 52 of the REACH Regulation.

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

Registrant(s)' commenting phase

ECHA received comments from you and forwarded them to the evaluating MSCA without delay.

The evaluating MSCA took the comments from you, which were sent within the commenting period, into account and they are reflected in the reasons (Appendix 1).

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

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

Subsequently, the evaluating MSCA received proposal(s) for amendment to the draft decision and modified the draft decision. They are reflected in the reasons (Appendix 1).

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

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

Your comments on the proposed amendment(s) were taken into account by the Member State Committee.

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MSC agreement seeking stage

The Member State Committee reached a unanimous agreement on the draft decision during its MSC-58 meeting and ECHA took the decision according to Article 52(2) and 51(6) of the REACH Regulation.

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Appendix 3: Further information, observations and technical guidance

1. This decision does not imply that the information provided by you in the registration(s) is in compliance with the REACH requirements. The decision neither prevents ECHA from initiating compliance checks on your dossier(s) at a later stage, nor does it prevent a subsequent decision under the current substance evaluation or a new substance evaluation process once the present substance evaluation has been completed.

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 relation to the required experimental studies on the isomer of the constituent DTBDA ppDTBDA **or** poDTBDA it is the responsibility of all the Registrant(s) to agree on the tested material to be subjected to the test(s) subject to this decision. The substance identity information of the sample tested must enable the evaluating MSCA and ECHA to confirm the relevance of the testing for the substance subject to substance evaluation.

4. In relation to the experimental stud(y/ies) the legal text foresees the sharing of information and costs between Registrant(s) (Article 53 of the REACH Regulation). You are therefore required to make every effort to reach an agreement regarding each experimental study for every endpoint as to who is to carry out the study on behalf of the other Registrant(s) and to inform ECHA accordingly within 90 days from the date of this decision under Article 53(1) of the REACH Regulation. This information should be submitted to ECHA using the following form stating the decision number above at:
https://comments.echa.europa.eu/comments_cms/SEDraftDecisionComments.aspx

   Further advice can be found at
http://echa.europa.eu/regulations/reach/registration/data-sharing. If ECHA is not informed of such agreement within 90 days, it will designate one of the Registrants to perform the stud(y/ies) on behalf of all of them.

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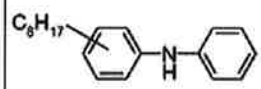
Appendix 4: Information related to Appendix 1: Reasons

Table 1: Chemical structure and QSAR estimations of relevant para/ortho substituted constituents of the registered substance regarding P, B and T screening information using COSMOmic 1504, EAWAG Pathway Prediction System, EPISuite and CHEMSPIDER.[6][7]

QSAR ESTIMATIONS ON P, B AND T SCREENING INFORMATIONS			
Nr	**Constituents**	**Structure**	
	[Group A] Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene		Mol weight = 281.3 g/mol (estimated) K_{oc} (MCI)= 4.401*10^4 L/kg (estimated) Log P_{ow} = 7.05 (estimated) S_w= 0.014 mg/L (estimated)
1	**Monotertoctyldiphenyl-amine** (para substituted [major part] and ortho substituted [minor part] isomers)		BCF (Regr.-based) =**12500** L/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF= **2667**/228700 L/kg (estimated) Biowin 2 (non-linear model): 0.0105 Biowin 3 (ultimate deg. Time): 2.0400 Biowin 6 (MITI-non-lin. Model):0.0119 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=0.0011 mg/L (estimated Daphnia, ChV=0.002 mg/L (estimated) Algea, ChV=0.023 mg/L (estimated)

[6] Note: The documentation of the QSAR results does not comply with REACH Annex XI, hence their reliability is limited. [a]ChV: Chronic Value.

[7] Note: The ECOSAR v1.11 and the BCFBAF v3.01 estimations have very high uncertainties regarding the predicted values for substances with a log Pow above 8 and 10, respectively.

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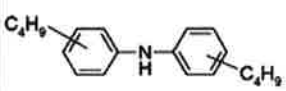
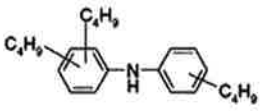
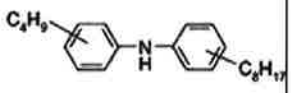
2	**[Group A]** Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene **Ditertbutyldiphenyl-amine** (para substituted [major part] and ortho substituted [minor part] isomers)		Mol weight = 281.3 g/mol (estimated) K_{oc} (MCI)= $3.894*10^4$ L/kg (estimated) Log P_{ow} = 7.11 (estimated) S_w= 0.014 mg/L (estimated) BCF (Regr.-based)= **11700** L/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF= **6761**/884500 L/kg (estimated) Biowin 2 (non-linear model): 0.0018 Biowin 3 (ultimate deg. Time): 2.0180 Biowin 6 (MITI-non-lin.Model): 0.0070 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=0.001 mg/L (estimated Daphnia, ChV=0.002 mg/L (estimated) Algea, ChV=0.021 mg/L (estimated)
3	**[Group B]** Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene **Tritertbutyldiphenyl-amine** (para substituted [major part] and ortho substituted [minor part] isomers)		Mol weight =337.4 g/mol (estimated) K_{oc} (MCI)= $2.729*10^5$ L/kg (estimated) Log P_{ow} = 8.96 (estimated) S_w=0.00015 mg/L (estimated) BCF (Regr.-based)= 1360 L/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF= 454/269700 L/kg (estimated) Biowin 2 (non-linear model): 0.0001 Biowin 3 (ultimate deg. Time): 1.6819 Biowin 6 (MITI-non-lin. Model):0.0020 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=<0.0001 mg/L (estimated) Daphnia, ChV=<0.0001mg/L (estimated) Algea, ChV=0.0018 mg/L (estimated)
4	**[Group B]** Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene **Monotertbutylmonotert-octyldiphenylamine** (para substituted [major part] and ortho substituted		Mol weight =337.4 g/mol (estimated) K_{oc} (MCI)= $3.022*10^5$ L/kg (estimated) Log P_{ow} = 9.02 (estimated) S_w= 0.00015 mg/L (estimated) BCF (Regr.-based) = 1450 L/kg(estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF= 534/316700 L/kg(estimated)

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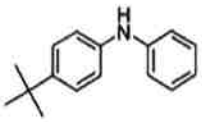
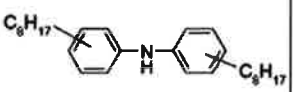
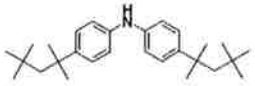
	[minor part] isomers)		Biowin 2 (non-linear model): 0.0001 Biowin 3 (ultimate deg. Time): 1.6819 Biowin 6 (MITI-non-lin. Model): 0.0033 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=<0.0001 mg/L (estimated) Daphnia, ChV=0.0002mg/L (estimated) Algea, ChV=0.00195 mg/L (estimated)
5	**Monotertbutyldiphenyl-amine** (CAS.: [redacted])		Mol weight = 225.2 g/mol (estimated) K_{oc} (MCI)= 5671 L/kg (estimated) Log P_{ow} = 5.20 (estimated) S_w= 1.16 mg/L (estimated) BCF (Regr.-based) = 1250 L/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF= 1840/3333 L/kg (estimated) Biowin 2 (non-linear model): 0.3507 Biowin 3 (ultimate deg. Time): 2.3761 Biowin 6 (MITI-non-lin. Model):0.0229 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=0.034 mg/L (estimated Daphnia, ChV=0.042 mg/L (estimated) Algea, ChV=0.241 mg/L (estimated)
	[Group C] Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene		Mol weight = 393.5 g/mol (estimated) K_{oc} (MCI)= $2.729*10^5$ L/kg (estimated) Log P_{ow} = 10.82 (estimated) S_w < 0.01 µg/L (estimated)
6	**Ditertoctyldiphenyl-amine** (para substituted [major part] and ortho substituted [minor part] isomers)		BCF (Regr.-based) =179 L/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF=17/10260 L/kg(estimated)
7	**Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N-[4-(1,1,3,3-tetramethylbutyl)-phenyl]** (CAS.: 15721-78-5)		Biowin 2 (non-linear model): 0.0000 Biowin 3 (ultimate deg. Time): 1.3458 Biowin 6 (MITI-non-lin. Model):0.0016 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=<0.0001 mg/L (estimated Daphnia, ChV=<0.0001mg/L (estimated) Algea, ChV=0.0002 mg/L (estimated)

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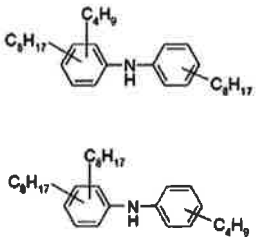
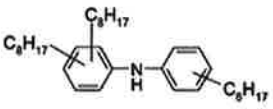
8	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene **Monotertbutylditert-octyldiphenylamine** (para substituted [major part] and ortho substituted [minor part] isomers)		Mol weight = 449.8 g/mol (estimated) K_{oc} (MCI)= *10^5 L/kg (estimated) Log P_{ow} = 12.73 (estimated) S_w < 0.01 µg/L (estimated) BCF (Regr.-based) =21 L/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF=1/813 L/kg (estimated) Biowin 2 (non-linear model): 0.0000 Biowin 3 (ultimate deg. Time): 1.0097 Biowin 6 (MITI-non-lin. Model):0.0004 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=<0.0001 mg/L (estimated Daphnia, ChV=<0.0001mg/L (estimated) Algea, ChV=<0.001 mg/L (estimated)
9	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene **Tritertoctyldiphenyl-amine** (para substituted [major part] and ortho substituted [minor part] isomers)		Mol weight = 505.7 g/mol (estimated) K_{oc} (MCI)= 1.276*10^8 l/kg (estimated) Log P_{ow} = 14.58 (estimated) S_w < 0.01 µg/L (estimated) BCF (Regr.-based)= 3 l/kg (estimated) Arnot-Gobas (lower trophic + biotransformation) BCF/BAF=1/3 l/kg (estimated) Biowin 2 (non-linear model): 0.0000 Biowin 3 (ultimate deg. Time): 0.6763 Biowin 6 (MITI-non-lin. Model):0.0002 Does not biodegrade fast/ not ready biodegradeable Fish, ChV=<0.0001 mg/l (estimated Daphnia, ChV=<0.0001mg/l (estimated) Algea, ChV=<0.0001 mg/l (estimated)