EUROPEAN CHEMICALS AGENCY

~~HIGHLY RESTRICTED~~

Decision number: CCH-D-0000004612-79-03/F Helsinki, 23 June 2014

DECISION ON A COMPLIANCE CHECK OF A REGISTRATION PURSUANT TO ARTICLE 41(3) OF REGULATION (EC) NO 1907/2006

For Phenol, dodecyl-, branched, CAS No 121158-58-5 (EC No 310-154-3), registration number: [redacted]

Addressee: [redacted]

The European Chemicals Agency (ECHA) has taken the following decision in accordance with the procedure set out in Articles 50 and 51 of Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH Regulation).

I. Procedure

Pursuant to Article 41(1) of the REACH Regulation ECHA has performed a compliance check of the registration for Phenol, dodecyl-, branched, CAS No 121158-58-5 (EC No 310-154-3), submitted by [redacted] (Registrant). The scope of this compliance check is limited to requirements regarding the identification of the substance (Section 2 of Annex VI). ECHA stresses that it has not checked any other information provided by the Registrant for compliance with REACH.

This decision is based on the registration as submitted with submission number [redacted], for the tonnage band of 1000 tonnes or more per year. This decision does not take into account any updates submitted after 6 March 2014, the date upon which ECHA notified its draft decision to the Competent Authorities of the Member States pursuant to Article 51(1) of the REACH Regulation.

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

The compliance check was initiated on 2 September 2013.

On 17 December 2013 ECHA sent the draft decision to the Registrant and invited him to provide comments within 45 days of the receipt of the draft decision.

By 31 January 2014 the Registrant did not provide any comments on the draft decision to ECHA.

On 6 March 2014 ECHA notified the Competent Authorities of the Member States of its draft decision and invited them pursuant to Article 51(1) of the REACH Regulation to submit proposals for amendment of the draft decision within 30 days of the receipt of the notification.

As no proposal for amendment was submitted, ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

II. Information required

A. Information in the technical dossier related to the identity of the substance

Pursuant to Articles 41(1)(a), 41(3), 10(a)(ii) and Annex VI, Section 2 of the REACH Regulation the Registrant shall submit the following information for the registered substance subject to the present decision:

1. Name or other identifier of the substance (Annex VI, 2.1.);
2. Composition of the substance (Annex VI, 2.3.)
3. Description of the analytical methods (Annex VI, 2.3.7)

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated registration to ECHA by **30 September 2014.**

III. Statement of reasons

Pursuant to Article 41(3) of the REACH Regulation, ECHA may require the Registrant to submit any information needed to bring the registration into compliance with the relevant information requirements.

A. Information in the technical dossier related to the identity of the substance

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

1. Name or other identifier of the substance (Annex VI, 2.1)

"Name or other identifier of the substance" is an information requirement as laid down in Annex VI, Section 2.1 of the REACH Regulation. The name and other identifiers are used to identify the substance in an unambiguous manner and are therefore fundamental for substance identification. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the Registrant identified the registered substance as of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). Information required to be provided on the naming of UVCB substances such as the registered substance shall consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process, as indicated in chapter 4.3 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.2, March 2012) - referred to as "the Guidance" thereinafter. ECHA observes that the Registrant did not provide sufficient and appropriate information on the naming of the registered substance (as indicated in point (i) and (ii) thereinafter).

(i). Chemical name

The Registrant assigned, as chemical name for the registered substance in the IUPAC name field in IUCLID section 1.1, "*phenol, alkyl branched (species comprising decyl, undecyl, dodecyl, tridecyl, tetradecyl, pentadecyl, substituents)*". Whilst this chemical name designates, in generic terms, six different groups of branched alkyl phenol constituents which are also reported by the Registrant in the composition, it does not accurately reflect the identity and predominance of the constituents actually present in the composition of the manufactured substance. In particular, according to the compositional information reported in IUCLID section 1.2, the C9 (branched) alkylphenols which are not quoted in the name can be present at a higher typical concentration level (ca. [redacted] %(w/w)) than the C15 (branched) alkylphenols quoted in the name and for which the typical contribution is ca. [redacted] %(w/w)). In addition, the current chemical name reported in the IUPAC name field in IUCLID section 1.1 does not specify the position of the branched alkyl substituents on the aromatic ring of these phenol derivatives.

ECHA observes that the Registrant recognised, in the description field of the reference substance in IUCLID section 1.1, that "*[a] more meaningful name to describe this UVCB substance*" could be provided and suggested for that purpose "*phenol, alkylation products with C10-C15 branched olefins derived from propene oligomerisation*". However, the suggested alternative chemical name does not specify the position of the alkyl substituent, nor does it provide a representative carbon number range for the branched alkyl substituent (as already explained above).

ECHA therefore concludes that the Registrant did not provide a representative chemical name for the registered substance.

The Registrant is accordingly required to revise the chemical name assigned to the registered substance as specified in the first bullet point of sub-section (iii) below.

(ii). The manufacturing process

ECHA observes that the Registrant provided a generic description of the manufacturing process in section 3.1 of the IUCLID dossier. According to this description, the registered UVCB substance is manufactured by reacting phenol and "[redacted]" under catalytic conditions and purifying the product from this reaction by a distillation step. However, this generic description is not considered sufficient to identify the registered substance, as explained thereinafter.

The compositional information currently provided by the Registrant in IUCLID section 1.2 of the dossier indicates that the registered substance consists of the following:

- A complex set of phenol-based constituents with an unspecific branched alkyl structure of carbon number varying from C9 up to at least C15. The position of these alkyl substituents on the phenol ring is also unspecified;
- Other groups of constituents such as unreacted starting materials, [redacted].

The composition of the registered substance is therefore expected to consist of a large number of constituents. As a result of the complexity in the composition, the registered UVCB substance can normally not be fully identified on the basis of its chemical composition alone without further detail on the manufacturing process, as explained in chapter 4.3 of the Guidance. The manufacturing process description to be provided shall normally consist of the chemical identity and ratio of the starting materials actually used and information on the most relevant steps of the manufacturing process and the associated process parameters, as also specified in chapter 4.3 of the Guidance. However, the registrant did not specify the following information:

- The ratio of reactants used in the process. This information may determine the level of alkylation of the phenol in the manufactured substance. The alkylation level however can currently not be derived from the reported composition, in line with the observations in section III.A.2 of this decision;
- Sufficient details on the identity of the "[redacted]" reactant used in the process. ECHA underlines that the composition of this starting material is one of the determinants of the composition of the registered substance. However, the current information provided in IUCLID section 1.2 of the registration dossier does not enable to establish the contribution of the "[redacted]" building blocks to the composition of the registered substance, in line with the observations in section III.A.2 of this decision;
- Further information on the processing parameters, such as the ion exchange resin type or any other relevant parameter, determining the relative abundance of the possible regioisomers (ortho-/meta-/para-) of the branched alkylphenol constituents in the registered substance. This information can currently not be derived from the reported composition, in line with the observations in section III.A.2 of this decision.

The Registrant is accordingly required to provide the missing information on the manufacturing process description, as specified under the second bullet point of sub-section (iii) below.

(iii). <u>The information required from the Registrant</u>

- <u>A chemical name representative of the registered substance must be provided.</u>

  Based on the observation set out in sub-section (i) above and pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant is required to revise the chemical name currently assigned to the registered substance. The chemical name shall reflect the identity (including the carbon number distribution) of the branched alkyl substituents as well as their position on the aromatic ring of the phenol constituents of the registered substance.
  Taking into account the following observations in the current registration dossier:

  - The declaration from the Registrant, in the Description field in IUCLID section 1.1, that the olefin starting material used in the process is characterised by the relative predominance of [redacted],
  - The indication that the substance may predominantly consist of para-alkylphenol isomers, as suggested by the proton Nuclear Magnetic Resonance (^{1}H NMR) spectrum, in particular the profile of the peaks from the aromatic protons observed in the 6.5-7.5 ppm region.

ECHA considers that, under these specific circumstances, "Phenol, alkylation products with C12-rich branched olefins from propene oligomerisation" is an appropriate chemical name for the registered substance.

- Further detail on the manufacturing process must be provided

Based on the observation set out in sub-section (ii) above and pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant shall specify the following information on the manufacturing process:

- Ratio of reactants;
- The overall composition of the [redacted] starting material, including the identity and upper and lower concentration levels of the constituents presenting the same carbon number and belonging to the same hydrocarbon class (e.g. branched alkenes);
- Specification of the processing parameters which determine the relative abundance of different alkylphenol regioisomers in the composition of the registered substance.

The Registrant shall ensure that the information is consistent throughout the dossier.

Regarding how to report the manufacturing process, the chemical name and manufacturing process description shall be specified in the "IUPAC name" and "Description" fields in IUCLID section 1.1, respectively.

2. Composition of the substance (Annex VI, 2.3)

"Composition of the substance" is an information requirement as laid down in Annex VI, Section 2.3. of the REACH Regulation. The substance composition corresponds to the chemical representation of what the substance consists of and is therefore an essential part of substance identification and the cornerstone of all the REACH obligations. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the composition reported in section 1.2 of the IUCLID dossier is not described to a sufficient level of detail and includes inapproriate information, as explained thereinafter:

- The Registrant reported, in IUCLID section 1.2 of the registration dossier, seven groups of mono-(branched alkyl)-substituted phenol constituents which differ from each other in terms of the carbon number of the branched alkyl group (from C9 to C15). ECHA observes that the reported composition does not provide any further information on the position of these branched alkyl groups on the phenol ring;
- The Registrant did not specify the upper and lower concentration level of the constituents reported in IUCLID section 1.2 of the registration dossier. Without this information, the variations in the composition of the registered substance cannot be established;
- The origin of the constituent "didodecylphenol", which refers to structures where the alkyl substituents on the phenol ring are linear, is ambiguous. In particular, the presence of such constituent would normally require the existence of significant amount of the linear dodec-1-ene in the "[redacted]" starting material. However, this starting material, as [redacted], is expected to predominantly consist of branched structures;

- The identifiers used for the constituents reported in the composition are not fully consistent across sections 1.2 and 1.4 of the IUCLID dossier. In particular, the EC and CAS identifiers assigned to the groups of constituents "didodecylphenol" refer to structures where the position of the alkyl substituents on the phenol ring is unspecific. However, the chemical name reported in the "IUPAC name" field and the assigned molecular and structural information specify that these alkyl substituents are in position ortho- and meta- of the phenol ring. The report from the chromatographic analysis attached in IUCLID section 1.4 of the dossier, for its part, refers to the presence of "2,4 didodecylphenol", i.e. a phenol with the alkyl substituents in position ortho- and para-.

ECHA therefore concludes that the composition currently reported in the dossier is not sufficient and appropriate for the identification of the registered substance.

According to chapter 4.3 of the Guidance, the Registrant shall note that, for UVCB substances such as the registered substance, the following applies:

- All constituents present in the substance with a concentration of ≥ 10 % shall be identified and reported individually;
- All known constituents and constituents relevant for the classification and/or PBT assessment of the registered substance shall be reported individually; and
- Unknown constituents or groups of constituents shall be identified as far as possible by a generic description of their chemical nature.

For each constituent and group of constituents, the minimum, maximum and typical concentration, shall be reported.

The Registrant is accordingly requested to specify, for each (branched alkyl)phenol group constituents presenting the same carbon number, the relative contribution in *ortho*-, meta- and *para*- isomers in the form of a range reflecting the variability observed in the composition. The registrant shall clarify the above mentioned inconsistencies or ambiguities on the identity of the "didodecylphenol" constituents. The Registrant shall also ensure to provide, for each constituent and group of constituents required to be reported, the typical, upper and lower concentration levels.

Therefore, pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: correct composition of the registered substance as specifically explained in the present decision.

Regarding how to report the composition in IUCLID, the following applies: The Registrant shall indicate the composition of the registered substance in IUCLID Section 1.2. For each constituent required to be reported individually, the IUPAC name, CAS name and CAS number (if available), molecular and structural formula, as well as the minimum, maximum and typical concentration, should be reported in the appropriate fields in IUCLID. For the other constituents to be reported under a generic description, a generic chemical name describing the group of constituents, generic molecular and structural information (if applicable), as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID. Regarding the reporting of the contribution of the *ortho*-, meta- and *para*- isomers of the alkylphenols already specified in the composition, the following shall apply as a baseline: the Registrant shall indicate the contribution of the relevant groups of isomers in the Remarks field of the repeatable block for each reported

alkylphenol in the form range. For example, where the regioisomers present are limited to the ortho- and para- isomers , the information can be reported in the form of a text such as "*para-/ortho-* ratio varies from [minimal ratio] to [maximal ratio]".

Further technical details on how to report the composition of UVCB substances in IUCLID are available in paragraphs 2.1 and 2.2.2 of the Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH (version: 2.0, July 2012) on the ECHA website.

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

"Description of the analytical methods" for the identification of the substance is an information requirement as laid down in Annex VI, Section 2.3.7 of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA observes that the Registrant did not provide sufficient description of the analytical methods used for the quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance, as requested according to annex VI section 2.3.7.

More specifically ECHA notes that the Registrant provided the report from a gas chromatographic (GC) analysis which includes a chromatogram and a peak list. The Registrant presented the results from this analysis in the form of a table listing 7 constituents and groups of constituents and the corresponding concentration values derived from this method. However, the quantification does not make a differentiation between the branched alkylphenols with carbon number C10, C11, C12, C13, C14 and C15 expected to be present in the composition, in line with the information reported in IUCLID section 1.1 and 1.2 of the registration dossier. The analytical report appears instead to present the overall concentration of these constituents under one generic entry referred to as "Phenol, dodecyl-, branched. Furthermore, this analytical method does not provide any quantitative information on the contribution of the ortho-, meta- and para-isomers within these branched alkylphenols.

ECHA therefore concludes that the description of the analytical methods used for the quantification of the constituents required to be reported is currently missing from the dossier.

Therefore, pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: description of the analytical methods used for the quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance.

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

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

The Registrant shall ensure that the composition reported in the dossier is consistent with the analytical results obtained.

IV. Information on right to appeal

An appeal may be brought against this decision to the Board of Appeal of ECHA under Article 51(8) of the REACH Regulation. Such an appeal shall be lodged within three months of receiving notification of this decision. Further information on the appeal procedure can be found on ECHA's internet page at http://echa.europa.eu/appeals/app_procedure_en.asp. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

[redacted]

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