EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004614-75-03/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 the 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 100 to 1000 tonnes 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. The spectral data (Annex VI, 2.3.5.)
4. Description of the analytical methods (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, dodecyl-, branched*". In the Remarks field of the reference substance in section 1.1, the Registrant added a statement (under the structural formula) indicating that the alkyl substituent on the phenol "*may be better described as C9/C10/11/12/13/14/15 branched alkyl, nominally referred to as "tetrapropenyl-derivatives*". The Registrant also specified, in the same IUCLID field, typical relative concentration values for the branched alkyl phenols according to the carbon number of the alkyl chain. According to this information, even though the C12 branched alkyl phenols typically represent the group of alkylphenol constituents with the highest concentration level, the branched C12 alkylphenols do not accurately reflect the identity and predominance of the branched alkylphenol constituents in the registered substance. In particular, the reported typical relative concentration level of the branched C12 alkylphenols remains below 80% and other constituents, such as branched C11 alkylphenols, exceed 10% and would therefore be expected to represent also predominant groups of constituents.

In addition, the analytical reports attached in section 1.4 designate the test substance as "*para-dodecylphenol*". According to this information, the representative position of the alkyl substituent on the phenol ring would therefore be para-. However, 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 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 information on the manufacturing process description which is limited to the identity of the starting materials used. In particular, the analytical report entitled "[redacted]" attached in IUCLID section 1.4 of the registration dossier, indicates that the starting materials used for the manufacturing are [redacted]". In addition, according to the structural information on the residual "[redacted]" reported in the composition, this starting material corresponds to an olefin. However, this description is not considered sufficient to identify the registered substance, as explained thereinafter.

The analytical information currently provided by the Registrant in IUCLID section 1.4 of the dossier indicates that the registered substance consists of the following:

- A complex set of phenol-based constituents and impurities with an alkyl branched structure of carbon number varying from below C9 (referred to as "light alkylphenols" by the Registrant) up to at least C15. These alkyl substituents can be both in ortho- and para- position on the phenol ring;
- 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. As a result, the following information is considered necessary for the identification of the substance:

- 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 composition of the olefin used, including the contribution of the "light" olefins ending up as "light alkylphenols" mentioned in the analytical report and the heavier olefins. The contribution of the light olefins can currently not be derived from the composition reported in the dossier. In addition, the variability in the concentration of the other olefin constituents is not specified in the dossier nor can it be derived from the reported concentration ranges of their reaction products with phenol, in line with the observations in section III.A.2 of this decision;
- Further information on the relevant processing steps (including any preliminary steps, the processing steps involving chemical transformations and any step applied for the purification and isolation of the registered substance) and associated processing parameters. Regarding the phenol alkylation step, specification of the parameters determining the relative abundance of para-alkylphenol constituents over the ortho-alkyl constituents (such as the catalysis type) shall be specified as a baseline. The Registrant shall note that the relative abundance of these groups of constituents can currently not be derived from the compositional information reported in the dossier, as explained in section III.A.2 of this decision;

The Registrant is accordingly required to provide the detailed description of the manufacturing process, 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 registration dossier:

- The indication in sections 1.2 and 1.4 of the IUCLID dossier that the registered substance is derived from the reaction between phenol and an olefin resulting from the oligomerisation of propene;

- The typical molecular and structural information of the registered substance which indicates that the olefin used in the manufacturing process is characterised by the relative predominance of C12 branched alkenes;

- The indication that the substance predominantly consists of para-alkylphenol isomers, as suggested by the results from analyses reported in IUCLID section 1.4.

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

- The detailed description of 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 provide a description of the manufacturing process and shall specify the following information:
- Ratio of reactants;
- the overall composition of the olefin starting material, including the identity and upper and lower concentration levels of the olefins presenting the same carbon number;
- Description of the relevant manufacturing processing steps and associated processing parameters.

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 does not include appropriate information for the identification of the registered substance.

More specifically, the Registrant reported the branched alkyl constituents under one generic entry using the chemical identifiers for "phenol, dodecyl-, branched". According to the information in the Remarks field of the reference substance for that group of constituents, branched alkylphenols with alkyl groups from C8 to C15 at an undefined position on the aromatic ring of the phenol (including at least ortho- and para- according to the analytical

information) can be covered by that entry. The Registrant also specified, in the same IUCLID field, the typical relative concentration level of these constituents according to the carbon number of the alkyl chain. However, no further information is provided on the concentration levels of the ortho- and para- isomers. In addition, the variability in the concentration levels of the branched alkylphenol isomers presenting the same carbon number has not been specified, except for "[redacted]" which has been reported separately. The contribution of "[redacted]" to the composition of the substance is itself ambiguous, since this group of constituents can also be covered by the generic group of constituents in the reference substance for "phenol, dodecyl-, branched".

In addition, the origin of the constituents "[redacted]" and "didodecylphenol", which refer to structures where the alkyl substituents on the phenol ring are linear, is ambiguous. In particular, the presence of such constituents would normally require the existence of significant amount of the linear dodec-1-ene in the "[redacted]" starting material. However, this starting material, as an "oligomer" of propylene, is expected to predominantly consist of branched structures.

Furthermore, the molecular and structural information for the constituents reported in the composition is also not fully consistent with the reported chemical name, EC or CAS information:

- The molecular and structural information for "didodecylphenol" indicates that the dodecyl substituents are in position ortho- and para- of the phenol ring while the assigned chemical name and EC and CAS entries do not specify the position of these substituents;
- The molecular and structural information for "[redacted]" indicates a specific branched structure (i.e. 7-methyloctyl-) while the assigned EC and CAS entries corresponds to a group of constituents with undefined branching;
- The molecular and structural information for "[redacted]" refers to dodec-1-ene while the assigned CAS entry refers to a group of constituents expected to be rich in C12 branched structures. The molecular and structural information furthermore does not reflect the existence of a carbon number distribution within these branched structures.

ECHA therefore concludes that the current composition includes insufficient and inappropriate information 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. The identification of these constituents must be provided for ECHA to establish the composition of the substance as manufactured and to use the compositional information as one identifier for the registered substance. For the substance which is the subject of this registration, the reporting of unknown branched alkylphenols according to groups

presenting the same carbon number and relative position of the alkyl substituent on the phenol ring is necessary as a baseline for this purpose.

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

Pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant is accordingly requested to provide the missing compositional information of the registered substance and clarify the above mentioned inconsistencies or ambiguities on the identity of the "[redacted]", "[redacted]", "[redacted]" and "[redacted]" constituents. The Registrant shall ensure that the information is consistent throughout the dossier.

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, shall 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 different alkylphenol constituents, the following shall apply as a baseline: the registrant shall report separately each group of alkylphenol presenting the same carbon number (e.g. "C15 branched alkylphenols") and specify the minimum, maximum and typical concentration for this group. For each alkylphenol group, the Registrant shall furthermore specify the contribution of the *ortho-* and *para-* isomers in the Remarks field of the corresponding repeatable block in the form of a range, 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. The spectral data (Annex VI, 2.3.5.)

"Spectral data" is an information requirement as laid down in Annex VI, Section 2.3.5. 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 registration does not contain the Ultra-Violet (UV) and Infra-Red (IR) spectral data required to support the identity of the registered substance. Reference to the existence of these spectral data has been included in the analytical report "[redacted]" attached in the dossier. According to the report, these spectra are available in "*appendix 4 and 6*". These appendices are however missing from the dossier.

ECHA points out that these spectra are a formal information requirement under Annex VI section 2.3.5. ECHA regards this required information scientifically relevant for the registered substance for the following reasons:

- The substance absorbs in the UV range due to the presence of chromophores in the composition. A UV spectrum representing the absorption of these constituents in the UV range can therefore be recorded;

- The IR spectrum displays characteristic vibration bands of covalent bonds in molecules present in the substance, including characteristic vibration bands from the chemical functionalities expected to be present in the composition.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the missing UV and IR spectral data as specifically explained above. The Registrant shall ensure that the information is consistent throughout the dossier.

As for the reporting of the spectral data in the registration dossier, the spectra shall be attached in IUCLID section 1.4.

4. 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 identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance, as specified in section III.A.2 of this decision.

ECHA notes that the provided chromatographic data (as *Appendix 5*) does not describe a method used for the quantification of the constituents in the substance. ECHA observes that reference is given to other chromatographic analyses are presented as quantitative analytical methods in the provided analytical report "[redacted]". However, the appendices given as reference (i.e. "Appendix1 & Appendix2") have themselves not been included in the dossier.

ECHA therefore concludes that the description of the analytical methods used for the quantification of the constituents and groups of 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 identification and 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 shall 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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