ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004610-83-03/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.

On 30 January 2014 ECHA received comments from the Registrant on the draft decision.

The ECHA Secretariat considered the Registrant's comments and, because the comments did not contain new technical information regarding the concerns raised in the draft decision, did not amend the draft decision.

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. Spectral data (Annex VI, 2.3.5)
4. Description of the analytical methods (Annex VI, 2.3.6 and 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 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 not 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, 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. It is also unclear how far the carbon number range C10-C15 is representative of the substance, the Registrant having declared in IUCLID section 1.1 that the substance is "*derived from a tetrapropene feedstock where C12 usually predominates (but often <[redacted]% mass)*".

ECHA observes that the Registrant recognised, in the description field of the reference substance in IUCLID, 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 still not accurately reflect the identity and predominance of the constituents actually present in the composition of the manufactured substance, 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 to remove water, excess of phenol and high molecular components. However, this generic description is not considered sufficient to identify the registered substance, as explained thereinafter.

The information currently provided by the Registrant on the structural formula in section 1.1 of the IUCLID dossier indicates that the registered substance consists of a complex set of phenol-based constituents with an alkyl branched structure of carbon number varying from C10 to C15. The provided gas chromatogram (GC) in IUCLID section 1.4 of the dossier, which shows a significant number of peaks, confirms the complexity of the substance. 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 and sufficient details on the composition of the "[redacted]" used. 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 building blocks from "[redacted]" in the constituents of the manufactured substance, in line with the observations in section III.A.2 of this decision;
- Further information on the processing parameters, such as the catalysis type, 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 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 C12 olefin constituents,
  - The indication that the substance may predominantly consist of para-alkylphenol isomers, as suggested by the Infra-Red (IR) spectral data reported in IUCLID section 1.4.

  ECHA considers that, under these specific circumstances, a chemical name such as "Phenol, *para*-alkylation products with C12-rich branched olefins from propene oligomerisation" can be considered appropriate 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 olefins presenting the same carbon number and ending up as light alkylphenols in the registered substance;
  - Description of the processing parameters which determine the relative abundance of para-alkylphenol constituents over the ortho-alkyl constituents.

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 registration does not contain sufficient information for establishing the composition of the specific registered substance and therefore its identity as required under Annex VI, 2.3 of the REACH regulation. More specifically, the Registrant reported, in IUCLID section 1.2 of the registration dossier, a composition corresponding to 100% w/w of the registered substance itself. Even though the generic chemical name assigned by the Registrant indicates that the registered substance includes branched alkylphenols where the branched alkyl structures comprise groups with carbon number C10, C11, C12, C13, C14 and C15, these six groups of constituents have not been reported individually. Furthermore, there is no qualitative and quantitative information on the regioisomers of these branched alkylphenols or on any other constituent or group of constituents eventually present in the composition.

ECHA therefore concludes that the composition has not been reported to the required level of detail. 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 specify the composition of the registered substance that is currently missing from the registration dossier.

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, 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 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. The Registrant shall also indicate the contribution of the relevant groups of regioisomers in the Remarks field of the repeatable block for each reported alkylphenol in the form of a 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. Spectral data (Annex VI, 2.3.5.)

"Spectral data" is a standard information requirement as laid down in Annex VI, Section 2.3.5. of the REACH Regulation. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA observes that the registration contains an IR spectrum. However the registration does not contain the Ultra-Violet (UV) and Nuclear Magnetic Resonance (NMR) spectra required to be provided according to Annex VI Section 2.3.5 of the REACH Regulation to support the identity of the registered substance.

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;
- NMR spectroscopic analyses such as a 1H-NMR or a 13C-NMR are powerful tools for structure characterisation and elucidation due to characteristic chemical shifts and spin-spin coupling which also reflect the relative abundance of individual atoms.

Pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant is therefore requested to submit a UV spectrum as well as a NMR spectrum, such as a ^{1}H-NMR or a ^{13}C-NMR. As an alternative to an NMR spectrum, mass spectra recorded as part of a mass spectroscopic analysis of the constituents in the registered substance can be provided.

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

The Registrant shall ensure that the description of the analytical methods used for the recording of the UV and NMR or MS spectra are specified in the dossier, in line with the requirements under Annex VI section 2.3.7.

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 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. However, the report does not include any description of a protocol followed to translate the results from the chromatographic analysis into concentration values of the group of constituents present in the registered substance. The method does not appear suitable to identify and quantify the branched alkylphenols with carbon number C10, C11, C12, C13, C14 and C15 expected to be present in the composition, including their regioisomers (ortho-, meta- and para-).

ECHA therefore concludes that the description of the analytical methods used for the quantification of the constituents and the results thereof 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.

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