ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 17 August 2018

Addressee [redacted]

Decision number: CCH-D-2114439549-36-01/F
Substance name: nonylphenol, ethoxylated
EC number: 500-024-6
CAS number: 9016-45-9
Registration number: [redacted]
Submission number: [redacted]
Submission date: 28/11/2012
Registered tonnage band: 1-10

DECISION ON A COMPLIANCE CHECK

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

1. **Name or other identifier of the substance (Annex VI, Section 2.1.);**
2. **Composition of the substance (Annex VI, Section 2.3.);**
3. **Spectral data (Annex VI, Section 2.3.5.);**
4. **High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.);**
5. **Description of the analytical methods (Annex VI, Section 2.3.7.).**

Taking into consideration the data currently available in the dossier and as explained in Appendix 1 to this decision, ECHA considers that the EC entry 500-024-6 (corresponding to "nonylphenol, ethoxylated"), which you assigned to the registered substance, describes a substance of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). Appendix 1 also specifies in detail all the information that ECHA considers appropriate in order to identify any UVCB substance. UVCB substances cannot be sufficiently identified by their chemical composition, because the number of constituents is relatively large; and/or the composition is, to a significant part, unknown; and/or the variability of composition is relatively large or poorly predictable. As a consequence, UVCB substances require other types of information for their identification, in addition to what is known about their chemical composition.

As a result, ECHA cannot be in a position, before receiving suitable information, to determine precisely the other types of information that are actually required to identify a specific UVCB substance. Only the Registrant of that UVCB substance knows the details of its identity. Based on this knowledge, he may consider that some of the information requested by ECHA is not suitable and necessary in order to identify the substance. Nevertheless, in that case it is the Registrant's exclusive responsibility 1) to ensure that

ECHA is in a position to identify precisely the substance and 2) to justify the reasons for which some information requested may have been omitted.

Therefore, if the Registrant eventually decides to submit only part of the detailed information specified in Appendix 1 to this decision and if the submitted information does not enable ECHA to establish and verify the identity of the substance actually covered by the dossier, the registration will not be considered valid.

You have to submit the requested information in an updated registration dossier by **26 November 2018** . You also have to update the chemical safety report, where relevant.

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

The scope of this compliance check decision is limited to the standard information requirements of Annex VI, Section 2 to the REACH Regulation.

Appeal

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

Authorised[1] by, Jos Mossink, Head of Unit, Substance Identification and Data Sharing, C2.

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

Appendix 1: Reasons

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

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

ECHA notes that you have not provided appropriate information on the name and other identifiers for the registered substance, as required according to Annex VI Section 2.1. of the REACH Regulation.

EC and CAS identifiers, the chemical name, as well as the other identifiers submitted, must describe precisely and consistently the identity of the registered substance.

You assigned the EC entry with EC number 500-024-6 and EC name "nonylphenol, ethoxylated" to the registered substance. This entry is included in the No-Longer Polymer (NLP) list (available on http://publications.jrc.ec.europa.eu/repository/bitstream/111111111/8721/1/6863%20-%20NLPFIN%20March1.pdf). It refers to a UVCB substance where the degree of ethoxylation is such that the substance is not a polymer (as defined in Article 3(5) of the REACH Regulation). It furthermore describes a substance which predominantly consists of constituents resulting from the [redacted], i.e. of a multi-constituent starting material where all the possible regioisomers ("[redacted]") are the main constituents. The reference to "[redacted]" indicates that the substituent on the phenol moiety is a [redacted] chain.

However, ECHA notes the following inconsistencies with the finding that the EC entry and EC name refer to a UVCB substance:

- You identified the registered substance as a **mono-constituent** substance and reported structural information describing mono-constituent substances. However, the identifiers corresponding to the submitted structural information would refer to different substances:
    - The reported structural formula corresponds to the substance having a [redacted] substitution of the phenol ring in the position [redacted] and showing one ethoxy unit bound to the hydroxyl group. The identifiers for this mono-constituent substance are EC# 248-762-5 (EC name '2-(nonylphenoxy)ethanol') and CAS# 27986-36-3.
    - The SMILES notation reported shows a [redacted] substitution of the phenol ring in the specific position [redacted] and showing one ethoxy unit bound to the hydroxyl group. The numerical identifier for this mono-constituent substance is CAS# 104-35-8 (the substance is not listed in the EC inventory).

  In line with the Guidance for identification and naming of substances under REACH (Version: 2.1, May 2017)- referred to as "the Guidance" hereinafter-, mono-constituent substances are well defined substances in which one constituent is

present at a concentration >80% (w/w) (referred to thereinafter as "main constituent"). A mono-constituent substance is named after the IUPAC name of its main constituent. Mono-constituent substances presenting different main constituents are considered different substances. Furthermore, mono-constituent substances and UVCBs are considered different substances under REACH.

- The chemical name "[redacted]" provided in the IUPAC name field in section 1.1 of the IUCLID dossier, describes in generic terms a substance including repeating units "[redacted]". This name does not specify further the level of ethoxylation of the substance and may refer to a **polymer** (as defined under Article 3(5) of the REACH Regulation) or to any other substance which does not meet the polymer definition (such as the No Longer Polymers with EC number EC 500-024-6). As a consequence this name does not specifically describe a unique UVCB substance and is not consistent with the EC identifier provided. Therefore the chemical name is not appropriate for the registered substance.

- The current CAS name "[redacted]" associated to CAS 9016-45-9 entry is the same as the chemical name you provided in the IUPAC name field. Therefore the discrepancies explained above for the chemical name can be drawn also for the CAS entry.

  ECHA also notes that, in the NLP list, the EC entry 500-024-6 is actually linked to CAS entry 9016-45-9. You shall however note that, as explained in the NLP list (page 8 of the document), "*NLP-Nos and name descriptions take precedence. The CAS-RN given are to be treated as indicative and for a use as a searching tool*".

  As a consequence, this entry does not specifically describe a unique UVCB substance and is therefore not appropriate for an unambiguous identification of the registered substance.

This information is therefore not consistent with the EC entry you assigned to the registered substance.

In light of the above discrepancies, ECHA concludes that the set of identifiers you assigned to the registered substance, including also the substance type you selected for your substance, present significant inconsistencies and therefore are overall inappropriate for its identification.

Accordingly, you are requested to provide consistent and appropriate identifiers for the registered substance.

- Chemical name:

  You are requested to specify a chemical name that is representative of the registered substance. You shall ensure that the chemical name reflects the exact identity of the substance subject to this registration and respects the naming conventions specified in the Guidance for the substance type your substance belongs to (mono-constituent substance, multi-constituent substance or UVCB).

- CAS entry:

  You are requested to delete the CAS (9016-45-9) information currently assigned to the substance and provide instead any available CAS information specifically corresponding to the substance. The CAS information needs to unambiguously describe the identity of the registered substance and should not represent any other substances than the registered substance. For example a mono-constituent substance where the main constituent shows a [redacted] substitution of the phenol ring in the specific position [redacted] and shows one ethoxy unit bound to the hydroxyl group would be appropriately described using CAS entry [redacted]. This CAS entry reflects the exact position (*4*-) and backbone type of the alkyl chain [redacted] bound to the phenol ring and also indicates the number of ethoxy units [redacted] Therefore the name: [redacted] defines the specific structure of the main constituent. Consequently, CAS entry [redacted] specifically corresponds to the described mono-constituent substance.

  You may however report the current CAS entry as "Other identifiers" in the registration dossier.

- EC entry:

  In case the current EC identifier is not appropriate to describe the registered substance, for technical reasons you should not remove or modify this EC entry when submitting the updated dossier, as the registration is linked to that EC entry in REACH-IT. To ensure unambiguous identification of the registered substance, you should however indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC number 500-024-6 currently assigned does not specifically correspond to the registered substance. This identifier cannot be modified or deleted at this stage in the present registration update for technical reasons". You should also specify, in the same "Remarks" field, any available and appropriate EC number for the substance.

  You should note that ECHA has established a process, subject to certain conditions, enabling registrants to adapt the EC identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned.

  Pending the resolution of the non-compliances addressed in the present decision, any possible adaptation of the identifier can only become effective once ECHA is in a position to establish unambiguously the identity of the substance intended to be covered by you with this registration. Should the information submitted by you as a result of the present decision enable ECHA to identify the substance unambiguously and result in a need to modify the identifier of the substance, the process of adapting the identifier will be considered relevant. In that case, ECHA will inform you in due time as to when and how the identifier adaptation process shall be initiated.

  In any case, you should note that the application of the process of adapting the identifier does not affect your obligation to fulfil the requirements specified in this decision.

- Description of the manufacturing process

If you decide, following the present decision, that the registered substance corresponds to a UVCB substance, you are reminded that, in line with chapter 4.3 of the Guidance, the description of the manufacturing process is required for its identification and shall normally consist in this case of the following:

- the identity and ratio of the starting materials used,
- a description of the most relevant steps taken during manufacturing affecting the composition and therefore the identity of the substance and the associated process parameters applied to those steps,
- Regarding more specifically the oligomerisation steps, you shall describe the parameters used to initiate, propagate and terminate the oligomerisation reactions,
- details and conditions applied for any isolation and purification steps.

ECHA underlines that, given the absence of appropriate compositional information on the registered substance (see Section 2 (Composition) hereinafter), and as the composition of the starting materials is to a significant extent known and is one of the factors determining the composition of the registered substance, compositional information of the starting materials is a necessary information for the identification of the registered substance itself as a baseline. The information to be provided shall include the overall ratio of the [redacted] and the alkyl backbone type (such as linear or branched) present in the [redacted] starting material used.

Accordingly, if the registered substance is a UVCB, you shall provide the above-mentioned information on the manufacturing process description.

You shall also ensure that the correct substance type (mono-constituent substance, multi-constituent substance or UVCB) is specified.

You shall also ensure that the molecular and structural information (including the SMILES notation and the structural formula that are requested to be provided according to Annex VI.2.2 of the REACH Regulation) are representative of the registered substance and are consistent with the name and other identifiers for that substance.

As for the reporting of the information in IUCLID:

- The chemical name should be specified in the "IUPAC name" field in IUCLID section 1.1.
- Any available CAS information should be reported under the CAS information header of the reference substance in IUCLID section 1.1. The CAS entry with CAS number 9016-45-9 can be reported under the "Other identifiers" field in section 1.1 of the IUCLID dossier.
- The manufacturing process description should be reported in the "Description of composition" field in section 1.2 of the IUCLID dossier.
- The substance type should be selected from the dropdown list under the "Type of substance" heading in IUCLID section 1.1.
- The structural information should be included in the "SMILES notation" and "Structural formula" field in IUCLID section 1.1.

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

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.

You assigned the EC 500-024-6 entry corresponding to "nonylphenol, ethoxylated" to the registered substance.

This entry describes a **UVCB substance** predominantly consisting of groups of constituents having [redacted] functional groups bound to phenyl rings in positions [redacted].

According to chapter 4.3 of the Guidance, 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 identified and reported individually;
- Unknown constituents shall be identified as far as possible by a generic description of their chemical nature;
- For each constituent/group of constituents required to be reported the minimum, maximum and typical concentration level shall be specified.

In spite of the above, you identified the registered substance as a mono-constituent substance in section 1.1 of the IUCLID dossier. According to chapter 4.2 of the Guidance, the following applies to all mono-constituent substances:

- A mono-constituent substance is a substance, defined by its quantitative composition, in which one main constituent is present to at least 80% (w/w);
- The main constituent shall be unambiguously identified by the chemical name and other relevant identifiers and shall be reported individually;
- All the impurities present at ≥ 1 % shall be identified and reported individually;
- All the impurities relevant for the classification and/or PBT assessment shall be identified and reported individually;
- For each constituent, including the main constituent and any impurity, the typical, minimum and maximum concentration level shall be specified.

ECHA notes that you reported a group of constituents described with the chemical name "[redacted]-". You also assigned EC 500-024-6 and CAS 9016-45-9 identifiers to this group of constituents. For this group of constituents only the typical concentration level is reported corresponding to [redacted]% (w/w). The identifiers indicate that the constituents include a linear (and therefore not branched) alkyl substituent on the phenol moiety.

The chemical name and EC and CAS identifiers reported are the same as the ones used for identifying the registered substance in section 1.1 of the IUCLID dossier.
As described hereinabove, in section 1 (Name or other identifier of the substance), these identifiers are inconsistent with each other and are inappropriate for describing the registered substance. Therefore, these identifiers are also inappropriate for describing the constituents present in the registered substance.

In addition, ECHA notes that with respect to the composition no further information is given in terms of:

- the concentration level of the constituents showing alkyl functional groups bound in different positions of the phenyl ring indicated in the chemical name. More specifically, no information is given on the presence and ratio of the [redacted].
- the concentration levels of the constituents having different [redacted] **levels**.
- the upper and lower concentration levels of the constituents/groups of constituents present in the registered substance.

Consequently, the information given on the constituents present in the registered substance is not consistent and lacks specifications on the identity of these constituents and related concentration levels.

If, following the present decision, you decide that the registered substance corresponds to a UVCB substance, you shall report the following:

- 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 identified and reported individually; and
- Unknown constituents shall be identified as far as possible by a generic description of their chemical nature. The identification of these unknown 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 substances such as ethoxylated 4-alkylphenols, the presence of unknown oligomeric constituents is only foreseen if the alkyl substituent displays undefined branching. In that case, a subdivision according to the degree of ethoxylation and the position of the alkyl substituent (e.g. 4-(branched nonyl)phenol mono-ethoxylate, 4-(branched nonyl)phenol di-ethoxylate...) is considered appropriate as a baseline;
- For each constituent or group of constituents, the typical, minimum and maximum concentration levels shall be specified.

  For substances such as "nonylphenol, ethoxylated", ECHA expects that the presence of individual nonylphenol ethoxylates (e.g. [redacted] is known...). These constituents should therefore be reported individually.

Alternatively if, following the present decision, you decide that the registered substance corresponds to a well-defined substance, the following applies:

- each main constituent (i.e. the constituent present at ≥80% for a mono-constituent substance or each constituent present at ≥10% and 80% for multi-

constituent substance) shall be identified and reported individually;
- All the impurities present at ≥ 1 % shall be identified and reported individually;
- All the impurities relevant for the classification and/or PBT assessment shall be identified and reported individually;
- For each constituent and impurity, the typical, minimum and maximum concentration levels shall be specified.

You are accordingly requested to correct the composition specified in the dossier so that the information specifically corresponds to the substance which is the subject of this registration.

Regarding how to report the composition in IUCLID, the following applies: you shall indicate the composition of the registered substance in IUCLID Section 1.2.

- If you decide to define the registered substance as a UVCB substance:

  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.

- If you decide to define the registered substance as a well-defined substance:

  For each constituent required to be reported, 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. Impurities shall be specified by at least one of the following identifiers: chemical name (IUPAC and/or CAS name), CAS-number and EC-number and/or molecular formula. The minimum, maximum and typical concentration shall be reported as well in the appropriate fields in IUCLID.

You shall ensure that correct molecular and structural identifiers are reported for each constituent/group of constituents and for each impurity in IUCLID section 1.2 as these are representative of the constituents present in the substance. You shall also ensure that the information provided on the composition of the substance is consistent with the identity of the registered substance and is confirmed by the analytical data included in section 1.4 of the IUCLID dossier.

Further technical details on how to report the composition in IUCLID are available in manual "How to prepare registration and PPORD dossiers" on the ECHA website.

3. Spectral data (Annex VI, Section 2.3.5.)

ECHA points out that the registration does not contain any spectral data which is required according to Annex VI, Section 2.3.5 of the REACH Regulation to support the indicated substance identity.

Instead, you gave a justification for not providing this information saying "*the quantitative and qualitative testings are still under testing*".

Beside the fact that the dossier was submitted in 2012 and never updated in that respect, ECHA points out that spectral data is a standard requirement of Annex VI, Section 2.3.5. ECHA regards the required spectral data as scientifically necessary for the identification of the registered substance for the following reasons:

- NMR spectroscopic analyses such as a ^{1}H-NMR or a ^{13}C-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. As the reported constituents contain characteristic hydrogen and carbon atoms, NMR is an appropriate analytical method to characterise the substance. In the case of a complex composition the NMR spectrum may not enable the structure of each constituent to be established, however it provides at least complementary information on the presence/absence of certain backbones and functionalities.

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

- 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.

Therefore, you are requested to submit UV and IR and NMR (such as a ^{1}H-NMR) spectra. As an alternative to the NMR spectrum, a mass spectrum of the registered substance can be provided.

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

4. High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.)

The registration does not contain any chromatographic data which is required according to Annex VI, Section 2.3.6 of the REACH Regulation to support the indicated substance identity.

Instead, you gave a justification for not providing this information saying "The quantitative and qualitative testings are still under testing".

Beside the fact that the dossier was submitted in 2012 and never updated in that respect, ECHA points out that this information is required since it constitutes a representation of the composition of the registered substance from the characteristic distribution of its constituents. Chromatographic methods are analytical methods commonly used for determining the concentration levels of the constituents/groups of constituents present in the composition of a substance. These methods maybe sufficient for that purpose or may be

used as a fingerprint or as complementary information to other analyses carried out for elucidating the composition of a substance.

Therefore you are requested to provide the report of a chromatographic analysis including a chromatogram, a peak list with the corresponding retention time and peak area.

You shall ensure that the description of the analytical method used for the chromatographic analysis, including the experimental set-up (i.e. the column type, length and diameter; injection volume; mobile phase/carrier gas; GC temperature programme; flow rate; concentrations of HPLC standard solutions; detection technique; and run time) and preparation of solutions and identity of standards, is specified, in line with the requirements of Annex VI section 2.3.7.

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

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

Description of the analytical methods is a formal information requirement of Annex VI Section 2.3.7 of the REACH Regulation.

This is also explained in section 4.1 of the Guidance: a description of the methods used for the identification of the substance and, where appropriate, for the identification of impurities and additives needs to be given. This information should be sufficient to allow the methods to be reproduced.

The information included in the analytical report needs to enable understanding how the constituents required to be reported in the composition section of the IUCLID dossier have been determined.

You did not provide any description of the methods used for determining the composition of the registered substance. Instead, you gave a justification for not providing this information saying "The quantitative and qualitative testings are still under testing".

As explained above such description is required according to Annex VI Section 2.3.7 of the REACH Regulation and is necessary for substantiating how the composition of the registered substance was determined.

You are therefore requested to provide the necessary description of the analytical methods for the identification and quantification of the constituents required to be reported in the composition information of the registered substance.

More specifically, you shall describe how you identified and quantified the constituents/groups of constituents present in the registered substance in terms of:

- The relative content of the different alkylphenols in terms of the backbone type (branched or linear) and position on the aromatic ring.
- The relative content of the groups of constituents presenting the same level of oligomerisation.

For this purpose, you shall provide an explanation on how the results of the analytical methods have been translated to the composition required to be reported in section 1.2, including peak tables, identification of the peaks, area percentages, and calculations used.

Taking into account the complexity of the composition of the registered substance, information on the identification and quantification of certain groups of constituents may be derived by combining information on the manufacturing process and results of the qualitative and quantitative analysis of the starting materials.

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

This information should be attached in IUCLID section 1.4 of the registration dossier.

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

The compliance check was initiated on 9 February 2017.

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

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

ECHA did not receive any comments by the end of the commenting period.

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

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

Appendix 3: Further information, observations and technical guidance

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

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