EUROPEAN CHEMICALS AGENCY

Helsinki, 20 October 2020

Addressees: [redacted]

Decision number: CCH-D-2114527134-58-01/F
Substance name: 4-Nonylphenol, ethoxylated
EC number: 500-045-0
CAS number: 26027-38-3
Registration number: [redacted]
Submission number subject to follow-up evaluation: [redacted]
Submission date subject to follow-up evaluation: 23 November 2018

DECISION TAKEN UNDER ARTICLE 42(1) OF THE REACH REGULATION

By decision CCH-D-2114439567-38-01/F of 16 August 2018 ("the original decision") ECHA requested you to submit information by 23 November 2018 in an update of your registration dossier.

Based on Article 42(1) of Regulation (EC) No 1907/2006 (REACH), ECHA examined the information you submitted with the registration update specified in the header above, and concludes that

Your registration still does not comply with the following information requirement(s):

1. **Composition of the substance (Annex VI, Section 2.3.);**

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

You are therefore still required to provide this information requested in the original decision.

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

The respective Member State competent authority (MSCA) and National enforcement authority (NEA) will be informed of this decision. They may consider enforcement actions to secure the implementation of the original decision and exercise the powers reserved to them under Article 126 of Regulation No 1907/2006 (penalties for non-compliance)[1].

In addition, ECHA notes that you failed to respond to the request "Name or other identifier of the substance (Annex VI, Section 2.1.)", which was contained in the original decision. This failure constitutes a direct infringement of the obligations arising under the original decision and of Article 41(4) of REACH. In principle, it is for the national enforcement authorities concerned to exercise the power reserved to it under Article 126 of REACH for the period during which the registration dossier was not compliant. As far as the request "Name or other identifier of the substance" is already directly enforceable, it is not reiterated in the present decision. Accordingly, the national enforcement authorities are competent to exercise their power both on requests 1 and 2 in the present decision and also on the request "Name or other identifier of the substance (Annex VI, Section 2.1.)", which you failed to addressed in

[1] See paragraphs 61 and 114 of the judgment of 8 May of the General Court of the European Court of Justice in Case T-283/15 Esso Raffinage v. ECHA

the original decision.

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, shall be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under http://echa.europa.eu/regulations/appeals.

Approved[2] under the authority of Christel Schilliger-Musset, Director of Hazard Assessment

[2] 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

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

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

Composition of the substance is an information requirement of Annex VI Section 2.3 of REACH.

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.

In the compliance check decision, you were 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.

In particular, the compliance check decision requested you

- to ensure that representative molecular and structural identifiers for each constituent/group of constituents and for each impurity are reported in IUCLID section 1.2.;

- to 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.

In your updated registration dossier, you identitifed the substance as a substance of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB) type.

In line with chapter 4.3 of the Guidance for identification and naming of substances under REACH (Version: 2.1, May 2017)- referred to as "the Guidance" hereinafter and as explained in the compliance check decision, for UVCB substances the following shall be reported::

- 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. 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 example, 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 [redacted] is considered appropriate;
- For each constituent or group of constituents, the typical, minimum and maximum concentration levels shall be specified.

In the updated registration dossier subject to follow-up evaluation, you have reported four constituents/groups of constituents:

1. The group of constituents identified as "4-nonylphenol, ethoxylated" (EC 500-045-0 and CAS 26027-38-3)
2. The constituent p-nonylphenol
3. The constituent ethylene oxide
4. A group of "unknown impurities"

ECHA observes the following:

4-nonylphenol, ethoxylated (EC 500-045-0 and CAS 26027-38-3):

- This group of constituent is identified by the same identifiers (EC, CAS and name) used to identify the registered substance, and are the same used in the previous submission of the registration dossier.

  EC and CAS identifiers, the chemical name, as well as the other identifiers, must describe precisely and consistently the identity of the groups of constituents present in the composition of the registered substance.

  EC entry 500-045-0 (associated to this reference substance) 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 ethoxylation of "4-nonylphenol", i.e. of a [redacted] The reference to "nonyl" indicates in this case that the substituent on the phenol moiety is a [redacted] chain.

  Therefore, this EC entry would be appropriate for describing a group of constituents showing [redacted] chains and differing one another because of their ethoxylation degree.

  However, ECHA notes the following:

  - You reported a SMILES notation and a molecular weight that would be appropriate for describing one single constituent having a [redacted] This information does not correspond to a group of constituents. This information is therefore not consistent with the EC entry you assigned to the group of constituents (and to the registered substance).

  - On the other hand, the CAS entry 26027-38-3 [redacted] describes in generic terms a substance including repeating units [redacted] This CAS entry does not specify further the level of ethoxylation 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 under REACH (such as the No Longer Polymer with EC number EC 500-045-0).

ECHA notes that, in the NLP list, the EC entry 500-045-0 is actually linked to CAS entry 26027-38-3. 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 explained above, this CAS entry does not specifically describe a unique UVCB substance and is therefore not appropriate for an unambiguous identification of the group of constituents present in the composition of the registered substance (and neither for the identification of the registered substance).

- In addition, ECHA observes that the NMR spectrum included in section 1.4 of the IUCLID dossier shows a [redacted] indicating the presence of a number of [redacted]. This indicates that the structure observed in the analysis includes [redacted].
  Such information is inconsistent with the information given on the group of constituents reported that is identified as having [redacted]

  Therefore, in light of the above discrepancies, ECHA concludes that the set of identifiers you assigned to the group of constituents presents significant inconsistencies, and therefore is overall inappropriate for the identification of the constituents present in the composition of the registered substance.

  Additionally, the compliance check decision explained also that for substances such as ethoxylated 4-alkylphenols, subdividing the groups of constituents according to the degree of ethoxylation (i.e. [redacted] is the appropriate way of reporting the composition.
  In the updated registration dossier you did not report information on the groups of constituents having different ethoxylation degree.

p-nonylphenol:

- The information given on the identity of the constituent p-nonylphenol indicates that the alkyl chain bound to the aromatic ring corresponds to a [redacted]
  Considering the manufacturing process description provided it is expected that this constituent corresponds to the starting material used for manufacturing the registered substance. As explained above, the NMR spectrum indicates instead the presence of [redacted].

  - In addition, there is no indication from the [redacted] that the registered substance would contain the [redacted] at the level as reported in IUCLID section 1.2 [redacted] Therefore, the information provided on the composition of the registered substance is not supported by the analytical data provided.

As explained above, the information provided in the updated registration dossier is neither consistent nor appropriate for describing the composition of the registered substance.

In conclusion you did not provide the information requested in the decision.

You are therefore still required to provide the information on the composition of the Substance.

In view of the deficiencies explained above, you shall report the following:

- Clarify the identity of the constituents present in the composition of the registered

substance reported as part of the group of constituents "4-nonylphenol, ethoxylated" in terms of the backbone type (branched/linear).

- Subdivide the reporting of the constituents/groups of constituents based on the ethoxylation degree. For substances such as ethoxylated 4-alkylphenols, a subdivision according to the degree of ethoxylation (e.g. [redacted] is considered appropriate. For each group of constituents the minimum and maximum concentration values shall be specified.

- Clarify the identity of the constituent "*p*-nonylphenol" in terms of the backbone type (branched/linear) and clarify the typical, upper and lower concentration levels of this constituent.

- Report the appropriate numerical identifiers and names for each constituents/group of constituents present in the composition of the registered substance. More specifically, the identifiers (chemical name, EC and CAS – if available) must specify the **position** of the alkyl chain on the phenolic ring nature and the **alkyl chain backbone type** (**branched or linear**). If the constituents of the registered substance have branched alkyl chains this needs to be reflected in the name and numerical identifiers. This is valid for all constituents/groups of constituents, including possible unreacted starting material (i.e. a clear identity of the starting materials should be provided in the description of the manufacturing process). In any case, the alkyl chain backbone type must be confirmed by the analytical data.

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 by creating for each constituent/group of constituents that is required to be reported a separate constituent record. 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.

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 ensure that the reporting of the compositional information is in line with the Guidance recommendations for UVCB substances. 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.

2. 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 REACH.

As 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. This means that the information included in the analytical report needs to be sufficient to verify the identity and quantity of the constituents reported in section 1.2 of the IUCLID dossier.

In the compliance check decision you were requested to describe how you identified and quantified the constituents/groups of constituents present in the registered substance in terms of:

- The relative content of the alkylphenol 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 were requested to provide an explanation on **how the results of the analytical methods have been translated to the composition** as reported in section 1.2, including peak tables, identification of the peaks, area percentages, and calculations used.

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.

In your updated registration dossier you provided a chromatographic report and spectral data. However, the reports provided do not include information on how you have derived the composition reported in section 1.2. Also no description of the protocol used for carrying out the analyses is included in the reports.

In addition, the NMR spectra provided are not supporting the compositional information reported in section 1.2 of the IUCLID dossier. As explained in section 2 (composition of the substance) of this decision,

- The spectra indicate the presence of [redacted] whereas the constituents reported have been identified as containing [redacted]
- Contrary to what is reported in the composition, the spectra do not indicate that the registered substance would contain significant concentration levels of [redacted] and at the same time significant concentration levels of the [redacted] starting material.
- The structural formula, molecular formula and molecular mass reported in the NMR spectrum report describe a substance having a [redacted] bound to the aromatic ring. This is not consistent with the name given for the registered substance describing [redacted]

Furthermore, the chromatographic report only indicates the presence of three main groups of constituents. The identification of the constituents behind these peaks has not been explained. In addition, there is no further break down of the composition documenting the concentration levels of the groups of constituents having different degree of ethoxylation.

In conclusion you did not provide the information requested in the decision.

You are therefore still required to provide the analytical information and relevant explanations as explained above.

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

Appendix 2: Procedural history

In accordance with Article 42(1) of the REACH Regulation, the Agency examined the information submitted by you in consequence of decision CCH-D-2114439567-38-01/F. The Agency considered that this information did not meet one or more of the requests contained in that decision. Therefore, a new decision-making process was initiated under Article 41 of the REACH Regulation.

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 of this decision was notified to the Member States Competent Authorities according to Article 51(1) of the REACH Regulation.

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 took into account your comment and did not amend the request(s).

The comment referring to cease of manufacture which does not relate to the content of this decision has been addressed in a separate communication to you.

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

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

Appendix 3: Further information, observations and technical guidance

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

2. The Article 42(2) notification for the original decision is on hold until all information requested in the original decision has been received.