Helsinki, 14 December 2016

Addressee: [redacted]

Decision number: CCH-D-2114350474-51-01/F
Substance name: Phenol, dodecyl-, sulfurized, carbonates, calcium salts
EC number: 272-233-8
CAS number: 68784-25-8
Registration number: [redacted]
Submission number: [redacted]
Submission date: 28.11.2010
Registered tonnage band: 100-1000T

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 (Annex VI, Section 2.1.) of the registered substance;**

2. **Composition (Annex VI, Section 2.3.) of the registered substance; and**

3. **Description of the analytical methods (Annex VI, Section 2.3.7) on the registered substance.**

You are required to submit the requested information in an updated registration dossier by **21 March 2017**. You shall also 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. Advice and further observations are provided in Appendix 3.

The scope of this compliance check decision is limited to the standard information requirement(s) of Annex VI, Section) 2 of 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, 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.

Authorised[1] by Leena Ylä-Mononen, Director of Evaluation

[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

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, Section 2.1.)

You identified the registered substance as of Unknown, or Variable Composition, or of Biological origin (UVCB substance) and you have assigned EC number 272-233-8 and CAS number 68784-25-8 corresponding to "Phenol, dodecyl-, sulfurized, carbonates, calcium salts" in section 1.1 of the IUCLID dossier.

EC and CAS identifiers must precisely describe the identity of the registered substance.

Information required to be provided according to Annex VI section 2.1 of the REACH Regulation on the naming of UVCB substances 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: 1.3, February 2014) - referred to as "the Guidance" thereinafter. In any case, the EC and CAS identifiers of shall also be specified (3).

(1) Chemical name

You provided a chemical name for the registered substance corresponding to "Phenol, dodecyl-, sulfurized, carbonates, calcium salts".

At the same time you reported information in the composition section of the registration dossier indicating the following:

- The substance contains ca. [redacted]% (w/w) of a group of constituents identified as "[redacted]".
- Ca. [redacted]% of a group of constituents identified by CAS entry [redacted] corresponding to "[redacted]" is present in the composition of the registered substance.
- [redacted] constituents have been reported and have been identified as "[redacted]". In addition in the remarks field of the corresponding reference substance it is stated that the "*substance is a UVCB [*[redacted]*]*".

ECHA notes the following:

- The chemical name provided does not take into account the presence of the oil "[redacted]" reported in section 1.2. ECHA points out that, unless the information required to be provided in the dossier demonstrates that the oil can be excluded to a significant extent from the composition, the identity of the oil shall be quoted in the name of the registered substance since it contributes to a significant level (>[redacted]% (w/w)) to its composition.

- The name used to identify the group of constituents "[redacted]" indicates that the composition of the registered substance includes constituents corresponding to derivatives of [redacted]. This information is inconsistent with the chemical name "Phenol, dodecyl-, sulfurized, carbonates, calcium salts" reported in section 1.1 that indicates instead that the [redacted] used as starting material correspond to [redacted].

[redacted] material, indicates that such starting material consists of [redacted]. However, the chemical name reported in section 1.1 for identifying the registered substance indicates that the [redacted] used corresponds only to a [redacted]

You are accordingly requested to ensure that the name reported in section 1.1 is representative for the substance which is the subject of the current registration and consistent with the information provided in other sections of the IUCLID dossier.

If "[redacted]" is a solvent that cannot be removed without affecting the stability of the substance, the presence of the solvent has to be reflected in the chemical name of the substance.

You should note the following in relation to the naming of your specific substance:

a) Alkyl groups

The chemical name shall reflect the exact identity of the [redacted] starting material used. In principle it is possible to construct the chemical name on the basis of:

- the main [redacted]: those [redacted] with a specific branched structure [redacted] if present, which individually have an upper concentration level ≥10% (w/w) in the starting material; and

- the [redacted] with groups of [redacted]), if present, which have an upper concentration level ≥10% (w/w) in the starting material.

However, this approach is considered appropriate only provided that the [redacted] altogether compose at least [redacted] % (w/w) of the substance.

If this condition is not met, all [redacted] constituents in the starting material, as identified by the carbon number and alkyl chain type (e.g. [redacted] substituent, shall be taken into account for the naming of that starting material.

Where the starting material is composed of one specific [redacted] at a concentration level of ≥80% (w/w), this starting material shall be designated, in the chemical name of the registered substance, by the chemical name of that [redacted].

b) Ratio of ortho/meta/para isomers

For the [redacted] starting material, the ratio of ortho/meta/para isomers shall be taken into account when designating the starting material in the substance name.

c) Degree of sulfurization and oligomerisation

Whenever a group of constituents presenting the same degree of sulfurization and oligomerisation is present at a concentration level of ≥80% (w/w) in the registered substance, that group shall be specified in the chemical name of the registered substance.

If such group does not exist, all the groups present at a concentration of ≥10% (w/w) designate the main group(s) to be referred to in the chemical name.

(2) Detailed description of the manufacturing process

Your registration includes a generic description of the manufacturing process in section 3.1 of the IUCLID dossier. The process description specifies:

"[redacted]"

ECHA notes that the specific identity of the starting materials used to produce the registered substance has not been described. You have stated that "[redacted]". However, further information on the identity and composition of the [redacted] starting material has not been provided.

Other elements of the manufacturing process description which are essential for the identification of the registered substance are also missing from the dossier. This concerns the ratio of starting materials used, specifications of any other relevant manufacturing process parameters, and any relevant isolation and purification steps have not been indicated.

Furthermore, you have stated that the substance is manufactured using a reaction with "[redacted] but no information has been provided on the levels of sulfurisation and oligomerisation, and on what process parameters lead to the desired levels of sulfurisation and oligomerisation.

ECHA therefore concludes that the manufacturing process has not been provided to a sufficient level of detail for the identification of the registered substance.

In line with the above observation, you are asked to provide the missing information on the manufacturing process description. This information shall include:

- the exact ratio of starting materials used in the process; and
- compositional information on the [redacted] starting material including
  - the upper and lower concentration levels of the (groups of) [redacted] constituents presenting the same carbon number, and
  - alkyl chain type (e.g. linear, branched)
  - ratio of ortho/meta/para isomers
- other relevant process parameters, including degree of sulfurization and oligomerisation
- Isolation and purification steps

The information provided must be sufficient to enable determining which alkyl groups (including the type of alkyl chain types such as linear/branched/cyclic, and carbon numbers such as C10, C11, C12, C13, C14 and C15) need to be reflected in the name of the substance.

(3) EC and CAS identifiers

You have assigned EC number 272-233-8 and CAS number 68784-25-8 corresponding to "Phenol, dodecyl-, sulfurized, carbonates, calcium salts" in section 1.1 of the IUCLID dossier.

These identifiers describe the same substance that is identified by the chemical name "Phenol, dodecyl-, sulfurized, carbonates, calcium salts" that you provided for the registered substance.

As explained hereinabove (under title (1) name) such name is not consistent with the information reported in the compositional section of the IUCLID dossier. Therefore the identifiers provided are also not consistent with the composition reported.

You are accordingly requested to ensure that the identifiers reported in section 1.1 are representative for the substance which is the subject of the current registration and consistent with the information provided in other sections of the IUCLID dossier.

As for the reporting of the information in IUCLID, the manufacturing process description shall be specified in the "Description of composition" field in IUCLID section 1.2. The chemical name shall be specified in the IUPAC name field in section 1.1.

If the CAS number is not appropriate to describe the substance which is the subject of the current registration, you shall delete from the dossier the CAS information currently assigned to the substance and provide instead any available CAS information specifically corresponding to the substance. If you deem it appropriate, you can however specify the current CAS information as "related CAS information" for the registered substance.

In case the current identifiers are not appropriate to describe the registered substance, you should not remove or modify at this stage this EC entry for technical reasons, the registration being 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 272-233-8 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. Any available CAS entry for the registered substance should be reported under the "CAS information" header of the reference substance in IUCLID section 1.1.

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.

Note:

The chemical name reported in section 1.1 indicates that both carbonates and calcium are present in the substance. If calcium carbonate is present in the substance, you should also provide representative structural formulae in section 1.1 that take into account the presence of carbonates in the substance. The information provided must be sufficient to enable determining whether the presence of these functionalities needs to be reflected in the name of the substance.

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.

According to Article 3(1) of the REACH Regulation, a substance is defined as a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition.

According to chapter 4.3 of the Guidance, for UVCB substances presenting a large number of constituents, 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 constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually; and
- Other constituents shall be identified 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 reported in the appropriate fields in IUCLID.

In the present dossier, you have reported the following groups of constituents:

[redacted]

The presence of other constituents was not indicated in the reported composition.

You did not report minimum and maximum concentration for the constituents (including the two last listed constituents that were reported as impurities) reported in section 1.2.

The information provided on each group of constituents does not fulfil the above mentioned information requirement for the following reasons.

a) "[redacted]

The constituents resulting from the chemical transformations are essentially reported under one main generic group (the first listed group of constituents) in the composition section of the IUCLID dossier. In relation to this group of constituents, "[redacted]", ECHA observes that the name provided indicates that this group consists of [redacted]. However, no further information has been provided on the identity of the constituents covered by this group of constituents.

ECHA notes that you have provided a representative structural formula that gives some information on the constituents covered by this group of constituents. The structural formula provided indicates that this group of constituents consists of dimers, trimers and tetramers including sulfur bridges consisting of up to three sulfur atoms.

Providing information in relation to the oligomerisation level and to the number of sulfur atoms present in the sulfur bridges is appropriate for describing substances such as the registered substance. However, you did not provide information on the concentration levels of the groups constituents presenting the same oligomerisation degree. You also did not provide information on the concentration levels of the constituents presenting different sulfur bridges.

In addition, no information has been provided on the upper and lower concentration levels of different [redacted] blocks presenting the same carbon number.

Furthermore the name "[redacted]" provided for this group of constituents includes the wording "[redacted]". However, the presence of "[redacted]" is not reflected in the structural formula provided. In addition no further information is given on the presence of "[redacted]" in this group of constituents.

ECHA therefore concludes that the identity and concentration of the constituents formed in the manufacturing of the registered substance have not been reported to a sufficient level of detail in the composition.

b) "[redacted]"

While the reported composition includes a significant amount of "[redacted]", the identity and concentration of the different constituents and groups of constituents present in the compostion of the oil have not been specified to a sufficient level of detail.

The description of the oil provided indicates that this oil consists of [redacted] having carbon numbers predominantly in the [redacted] range and contains a relatively large proportion of [redacted]. However, the dossier does not include any qualitative and quantitative information on the different [redacted] classes including linear alkanes, branched alkanes, cycloalkanes, their unsaturated counterparts, and the aromatic constituents presenting different number of aromatic cycles (mono-, di-, tri-,...) and on the carbon number distribution within each of these classes.

According to the substance definition given in Article 3(1) of the REACH Regulation described hereinabove, you shall note the following:

To the extent that the quantity of "[redacted]" reported in the composition is not a solvent which can be removed without affecting the stability of the substance or changing its composition, its constituents shall be regarded as constituents of the registered substance. Accordingly, if the solvent is present in the substance in significant concentration levels, the identity and concentration level of the constituents and groups of constituents originating from this solvent need to be specified to reflect as far as possible the actual identity of the solvent. This information has not been reported in section 1.2 of the IUCLID dossier.
If "[redacted]" is a solvent that cannot be removed without affecting the stability of the substance, its

identification 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.

c) "[redacted]

[redacted] constituents have been identified as "[redacted]" in section 1.2 of the IUCLID dossier. This name describes constituents having [redacted] alkyl chains.

However in the remarks field of the corresponding reference substance it is stated that "The substance is a UVCB [[redacted]]". This information indicates that such starting material consists of [redacted].

Therefore this information is inconsistent with the name provided for this group of constituents.

ECHA therefore concludes that the compositional information has not been provided to the required level of detail.

You are accordingly requested to complete and correct the information provided on the composition of the registered substance. You shall report:

- All constituents present in the substance with a concentration of ≥ 10 %;
- All constituents relevant for the classification and/or PBT assessment of the substance, and
- Other constituents shall be identified by a generic description of their chemical nature. The identification of these other 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 groups of constituents that correspond to [redacted], the following information is required:

    - The overall ratio of ortho/meta/para isomers.
    - Relative content of the different [redacted] derivatives according to the carbon number of the alkyl chain and according to the backbone type (branched/linear).
    - Relative content of dimers, trimers and tetramers
    - Quantitative information on constituents presenting different sulfur bridges.

  - For the [redacted] constituents originating from the "[redacted]", the reporting of the different [redacted] classes including linear alkanes, branched alkanes, cycloalkanes, their unsaturated counterparts, and the aromatic groups of constituents presenting different number of aromatic cycles (mono-, di-, tri-,...) is necessary as a baseline for ECHA to establish the composition of the substance. For each group of constituents, quantitative information on the carbon number distribution shall also be specified to conclude on the compositional profile of the constituents within the group.
    In addition any specific constituent that is relevant for the classification and/or PBT assessment of the substance shall be reported.

If "[redacted]" contributes extensively to the composition the chemical name of the registered substance shall refer to the presence of "[redacted]" to reflect as far as possible its actual identity.

In addition you shall clarify the inconsistency of the information given for the group of constituents "[redacted]". More specifically you shall clarify the identity of the constituents present in this group in relation to the carbon chain length.

You shall ensure that the reported composition is consistent with the description of the process used for the manufacturing of the registered substance, including the identity of the starting materials used. You shall also ensure that the composition is verifiable and therefore supported by a description of the analytical methods for the quantification of the constituents required to be reported, as required under Annex VI, section 2.3.7.

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.

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.

Information on the relative content of the different [redacted] derivatives within the relevant groups of constituents shall be specified in the Remarks field of the reference substance for that group.

Further technical details on how to report the composition of well-defined substances in IUCLID are available in the Manual "How to prepare registration and PPORD dossiers" on the ECHA website.

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

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

According to Annex VI Section 2 of the REACH Regulation, for each substance, the information given in this section shall be sufficient to enable each substance to be identified. This means that 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 identified and quantified.

You have provided an analytical report in section 1.4 of the IUCLID dossier in support of the composition of the registered substance. The reported composition includes:

- a group of constituents corresponding to [redacted]" and
- a group of constituents corresponding to "[redacted]" and
- a group of constituents corresponding to "[redacted]".

ECHA notes the following in relation to the analytical report provided:

- The provided chromatographic analysis cannot be used as such to draw any conclusion on the composition of the registered substance. A HPLC chromatogram (HPLC-OLOA 218A.pdf) was provided but the peak table is missing and peaks have not been identified. The analytical report does not include any information as to how the results from the chromatographic analysis have been translated into concentrations of the constituents listed in section 1.2. Moreover, the report does not include any description of the experimental procedure used to derive this information from the chromatogram.

- The provided methods together with the interpretation of the results do not provide sufficient information on the relative content of the different [redacted] in terms of the carbon chain length, backbone type and position on the aromatic ring.

- The structural information provided in section 1.2 for reference substance "[redacted]" indicates that your substance consists of "[redacted]". In addition the structural formula shows the presence of sulfur bridges.

  However, you have not provided information that enables ECHA to conclude that the [redacted] present in the composition of the registered substance consist of the "[redacted]"

  In addition no information is given on how you concluded on the number of sulfur atoms in the sulfur bridges indicated in the structural formula.

  It should be highlighted that, for you to meet these information requirements, ECHA would consider on the case-by-case any method that would be suitable support the declared composition. The methods to be considered by you are therefore not limited to analyses carried out on the registered substance but can also be based on considerations regarding i.a. the manufacturing process, analyses of the starting materials and derivatisation.

- If "[redacted]" is a solvent that cannot be removed without affecting the stability of the substance, the description of the analytical method used to determine the chemical nature of the solvent and its composition has to be provided.

- The chemical name "[redacted]" reported in section 1.1 indicates that both carbonates and calcium are present in the substance.
    - No analytical information is given in relation to these elements of the composition of the registered substance.
    - Furthermore, you have not provided a description of the analytical methods to identify the calcium counter-ion.

Therefore, the information provided is not sufficient to support the identification and the quantification of the constituents and groups of constituents required to be reported in the IUCLID dossier.

You are accordingly requested to provide a 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.

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 [redacted] in terms of the carbon chain length, backbone type and position on the aromatic ring.
- The relative content of the groups of constituents presenting the same level of oligomerisation.
- The relative abundance of sulfur bridges having the same number of sulfur atoms.
- Carbonates and calcium counter-ion that are present in the substance.
- Chemical nature of the solvent and its composition, if the solvent "[redacted]" cannot be removed without affecting the stability of the substance.

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.

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.

Taking into account the complexity of the composition of the registered substance, information on the identification and quantification of its 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.

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

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 **10 August 2016**.

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 request(s) in this decision, or to fulfil otherwise the information requirement(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.