EUROPEAN CHEMICALS AGENCY

Helsinki, 10 August 2017

Addressee: [redacted]

Decision number: CCH-D-2114366509-38-01/F
Substance name: benzenesulfonic acid, mono-c16-24-alkyl derivs., calcium salts
EC number: 274-263-7
CAS number: 70024-69-0
Registration number: [redacted]
Submission number: [redacted]
Submission date: 25.05.2016
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;**
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);**

You are required to submit the requested information in an updated registration dossier by **17 November 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 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.

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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.)

Information required to be provided according to Annex VI section 2.1 of the REACH Regulation 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: 1.4, June 2016) - referred to as "the SID Guidance" hereinafter.

According to the SID Guidance, the description of the manufacturing process shall include information on the chemical identity of the starting materials and information on the most relevant steps of the process. The consequence of defining a substance as UVCB is that any significant change of source or process would be likely to lead to a different substance.

You provided in IUCLID section 1.1 for the substance the EC and CAS numbers 274-263-7 and 70024-69-0, respectively, corresponding to "*Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts*". In the IUPAC name field you provided the chemical name "[redacted]".

You provided the following manufacturing process description in section 3.1 of the IUCLID dossier: "[redacted]."

In the "Description" field in section 1.1 you indicated that "[redacted]".

Information on the "[redacted]" used in the manufacture was provided in section 1.4 in the analytical report attachments, as explained in more detail below in section 2 of this Appendix in relation to the "Composition of the substance". Several different [redacted] were reported in the attachments with acronyms ("[redacted]"), however, no information on the exact identities and compositions of the [redacted] was provided.

However, ECHA notes that you did not specify the exact identity and composition of the [redacted] which is indicated as starting material in the manufacturing process, although in the "Description" you indicated that information on the starting material composition is available from the supplier. As the composition of the starting materials is an important factor determining the composition of the registered substance, it is a necessary element for the identification of the registered substance itself.

The identity/identities of the "[redacted]" are/is unclear as only acronyms were provided for their identification. No information was provided on the EC and CAS identifiers of the [redacted] or on their compositions. The [redacted] was/were not reported in the composition in section 1.2 in the IUCLID dossier. Although it was mentioned in the attachments in IUCLID section 1.4 that [redacted] cannot be removed, there was no scientific justification included in the dossier for this. Therefore, also the role and the amount of the [redacted] in the substance is not clear.

Similarly, no information was provided on the identity of the [redacted]

Furthermore, the description of the manufacturing process included in IUCLID Section 3.1 does not contain any indication on the ratio of reactants and does not specify the manufacturing process parameters (such as temperature and pressure) which are necessary to obtain the registered substance. Specification of the ratio of reactants and identification of process steps and process parameters that may affect the substance composition is essential for the identification of the registered substance.

In the manufacturing process you described that "[redacted]". However, it has not been described if the addition or non-addition of [redacted] during the process affects the substance composition: e.g. the addition of [redacted] may lead to formation of [redacted] in the substance, and potentially to an "overbased" substance where there is excess of [redacted]. It is noted that there is a separate CAS number for the overbased analogue of the registered substance: [redacted]. In this context it should be highlighted that, in general for UVCB substances, any significant change of source or process would be likely to lead to a different substance. However, in the absence of further information it cannot be concluded if the addition or non-addition of [redacted] would be considered as a significant change in process.

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

Therefore, you shall provide the missing information on the manufacturing process description. This information shall include:

- The exact identities and ratios of the starting materials and auxiliary agents used in the process (auxiliary agents including e.g. the "[redacted]
- Compositional information on the [redacted] acid starting material including:
    - the upper and lower concentration levels of the (groups of) constituents presenting the same carbon number, and
    - alkyl chain type (e.g. linear, branched; if relevant)
    - ratio of ortho/meta/para isomers
- Role, identities and compositions of the "[redacted]", as relevant:
    - Role: as explained in more detail below in section 2 of this Appendix in relation to the "Composition of the substance",
    - Identifiers: EC/CAS identifiers and chemical name(s),

  - Composition: as explained in more detail below in section 2 of this Appendix in relation to the "Composition of the substance";
- Explanation on the effect of adding or not adding [redacted] during the manufacturing process;
- Specifications of all relevant process parameters, including temperature and pressure values, and any other process steps and their parameters including purification step(s) (if any) which are necessary to obtain the registered substance and which may affect the substance composition.

If the currently provided chemical name is not appropriate for the substance, it shall be revised considering:

- Alkyl chains in the [redacted]: Carbon number distribution, alkyl chain type, ortho/meta/para isomer distribution (as relevant)
- [redacted]: The [redacted] has not been reported in the composition in section 1.2. Also, the current EC and CAS identifiers and the chemical name of the substance do not take into account the [redacted]. 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 chemical name of the registered substance if it contributes to a significant level to its composition.
- Carbon dioxide: It should be considered whether the adding or not adding [redacted] affects the substance identity and thus the chemical name.

As for the reporting of the information in IUCLID 6, the manufacturing process description for the registered substance shall be reported in the "Description of composition" field in IUCLID 6 section 1.2.

All information in the dossier needs to refer consistently to one substance.

If there is the need to revise the chemical name, and the current EC and CAS identifiers do not sufficiently describe the composition and identity of the substance, you shall:

- Report the appropriate chemical name 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 the EC entry 274-263-7 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 274-263-7 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.

Further technical details on how to report the identifiers of UVCB substances in IUCLID 6 are available in the Manual "How to prepare registration and PPORD dossiers" on the ECHA website.

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

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 SID 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.

Furthermore 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, should be reported in the appropriate fields in IUCLID.

In the registration dossier you have identified the registered substance as a UVCB substance and specified in IUCLID section 1.2 that the substance contains [redacted]% of the registered substance "[redacted]". You provided the following description for this generic group of constituents: "[redacted]".

The manufacturing process included in IUCLID section 3.1 mentions that the substance is manufactured in the presence of [redacted], and the analytical information included in section 1.4 shows the presence of [redacted] in the substance. You have explained e.g. in the attachment "[redacted] that [redacted]".

However, you did not report any [redacted] in the composition in section 1.2. In the Chemical safety report attached in IUCLID section 13 you have made the following statement in relation to the Physical state of the substance: "*The [redacted] is not, however, a constituent of the substance.*"

The information provided on the composition does not fulfil the above mentioned information requirement for the following reasons.

(1) Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts

The constituents resulting from the chemical transformations are essentially reported under this generic group in the composition section of the IUCLID dossier. Additional information was provided in the remarks indicating that the alkyl chains would be linear, saturated chains. However, no further information has been provided on the identity of the constituents covered by this group of constituents, e.g. no information was provided on the upper and lower concentration levels of different alkylbenzenesulfonate blocks presenting the same carbon number, or on the ratios of ortho/meta/para isomers. In the description you referred to the complexity of the substance "[redacted]".
In consequence, it may not be possible to provide detailed information on constituents and the composition of the substance on the basis of analysing the registered substance. In such case, in order to enable the identification of the substance, you should compensate this lack of information by providing information on composition in section 1.2 of the IUCLID dossier on the basis of the manufacturing process and the starting materials composition.

[redacted]

In principle, if the [redacted] cannot be removed from the substance without changing the composition, it becomes part of the substance and needs to be reported as a constituent in section 1.2. Only solvents which can be removed from the substance can be considered to not be part of the substance.

[redacted]

Furthermore, the manufacturing process reported in section 3.1 indicates that [redacted] and in some cases [redacted] are used in the process. This may lead to formation of [redacted] in the substance. If [redacted] is present in the substance, you need to report it in section 1.2 with its typical, minimum and maximum concentrations.

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 constituents/groups of constituents that correspond to "Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts", the following information is required:

- The overall ratio of ortho/meta/para isomers;
- Relative content of the different alkyl benzenesulfonate derivatives according to the carbon number of the alkyl chain, and if relevant, according to the carbon backbone type (branched/linear);
- Information on any other (groups of) constituents required to be reported in section 1.2.

For the [redacted] the following is required:

- If the [redacted] cannot be removed from the substance, you shall report the oil in section 1.2 with the appropriate identifiers (EC, CAS, chemical name) and including the minimum amount of oil that is required in order not to change the composition;
- Clarification on if the different acronyms reported in the analytical data refer to different [redacted];
- For the hydrocarbon constituents originating from the "[redacted]" the reporting of the different hydrocarbon 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. For each "[redacted]" used in the manufacture of the substance this information shall be given separately.

The information shall be included in section 1.2 of the registration dossier.

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., including the results from these methods. Considering the complexity of the substance, (additional) compositional information can be provided on the basis of the starting materials composition and the manufacturing process.

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

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

According to Annex VI Section 2.3.5 of the REACH Regulation, spectral data (ultra-violet spectrum, infra-red spectrum, as well as nuclear magnetic resonance or mass spectra) is required to be reported in a registration dossier and this information is required to be sufficient to enable the identity of the substance to be verified.

You provided UV-vis, IR, NMR and MS spectral data in the registration dossier. However, the spectral data have been recorded on a sample diluted with [redacted].

The spectral data is insufficient to identify the registered substance due to the fact the substance is heavily diluted in [redacted]. Although you mention that the removal of the [redacted] is not possible, there is no scientific justification provided for this.

You shall ensure that the identification of the registered substance is based on the information for the substance as such and not the substance in a mixture. You shall note that the [redacted] which can be removed from the substance without affecting its stability or changing its composition shall be removed before generating the spectral data.

You shall provide spectral data for the registered substance as such. This includes an ultra-violet spectrum, infra-red spectrum, as well as nuclear magnetic resonance or mass spectra.

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

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

According to Annex VI, section 2.3.6 of the REACH Regulation, the registration needs to contain a high-pressure liquid chromatogram (HPLC) or a gas chromatogram (GC).

You provided in section 1.4 results of LCMS-MS and electrospray MS analyses in the attachments "[redacted]" and "[redacted]". However, only MS fingerprints are included from these measurements, but no chromatograms, peak tables or quantification based on the results was provided. Also, no other alternative quantification results were provided.

The provided information is not sufficient to fulfil the information requirement as you have not included any chromatogram in the registration dossier.

Therefore, you are requested to submit a GC or an HPLC chromatogram and the required chromatographic data (retention times, peak areas/results and quantifications) that supports the identification and/or quantification of the substance.

You shall ensure that the description of the analytical methods used for the recording of the chromatographic data is specified in the dossier, in line with the requirements under Annex VI section 2.3.7. This information 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.

The information shall be included in section 1.4 of the registration dossier.

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

According to Annex VI, section 2.3.7 of the REACH Regulation, a registration dossier shall report a description of the analytical methods or the appropriate bibliographic references for the identification of the substance and where appropriate for the identification of impurities and additives. The reporting shall be given in sufficient detail that the methods may be reproduced.

You provided only spectral data (including IR, UV, H-NMR spectra and the mass spectrum) in IUCLID section 1.4, whereas you did not provide any quantification of the composition of the substance.

The spectral data alone is not sufficient to verify the composition of the registered substance.
You are requested to provide a detailed description of the analytical method(s), and the corresponding results, used for the quantification of the registered substance. Information shall be provided on:

- Identification and quantification of the (groups of) constituents included in the generic constituent "Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts", and required to be reported in the composition in section 1.2;
- If "[redacted]" cannot be removed without affecting the composition or stability of the substance, the description of the analytical method, and the results thereof, used to determine the chemical nature of the oil and its composition has to be provided.
- Overall quantity of the [redacted] which cannot be removed without affecting the stability of the substance or changing its composition;
- Identification and quantification of the calcium counter-ion;
- Content of calcium carbonate (if present);
- Any other constituents required to be reported in the composition of the registered substance

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.

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.

For quantification methods based on chromatography, the information shall include a legible print-out of the chromatogram as well as the report from the chromatographic analysis including the table of peak assignments that report the peak areas and corresponding amounts of each relevant constituent/impurity.

In addition, you shall ensure that the composition reported in IUCLID section 1.2 is in line with the information provided in section 1.4, which shall be sufficient to identify and quantify the substance.

The information shall be included in 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 13 April 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.