

Decision number: CCH-D-0000004593-71-03/F

Helsinki, 31 July 2014

**DECISION ON A COMPLIANCE CHECK OF A REGISTRATION PURSUANT TO ARTICLE 41(3) OF REGULATION (EC) NO 1907/2006****For Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs., CAS No 85536-14-7 (EC No 287-494-3), registration number: [REDACTED]****Addressee:** [REDACTED]

The European Chemicals Agency (ECHA) has taken the following decision in accordance with the procedure set out in Articles 50 and 51 of Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH Regulation).

**I. Procedure**

Pursuant to Article 41(1) of the REACH Regulation ECHA has performed a compliance check of the registration for Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs., CAS No 85536-14-7 (EC No 287-494-3), submitted by [REDACTED] (Registrant). The scope of this compliance check is limited to the standard information requirements of Annex VI, Section 2 of the REACH Regulation.

This decision is based on the registration as submitted with submission number [REDACTED], for the tonnage band of 1000 tonnes or more tonnes per year. This decision does not take into account any updates submitted after 6 March 2014, the date upon which ECHA notified its draft decision to the Competent Authorities of the Member States pursuant to Article 51(1) of the REACH Regulation.

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

The compliance check was initiated on 29 October 2013.

On 19 December 2013 ECHA sent the draft decision to the Registrant and invited him to provide comments within 45 days of the receipt of the draft decision. That draft decision was based on submission number [REDACTED].

By 3 February 2014 the Registrant did not provide any comments on the draft decision to ECHA.

On 6 March 2014 ECHA notified the Competent Authorities of the Member States of its draft decision and invited them pursuant to Article 51(1) of the REACH Regulation to submit proposals for amendment of the draft decision within 30 days of the receipt of the notification.

As no proposal for amendment was submitted, ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

## II. Information required

### 1. Information in the technical dossier related to the identity of the substance

Pursuant to Articles 41(1), 41(3), 10(a)(ii) and Annex VI, Section 2 of the REACH Regulation the Registrant shall submit the following information for the registered substance subject to the present decision:

1. Name or other identifier of the substance (Annex VI, 2.1.), as further specified under section III.A.1;
2. Composition of the substance (Annex VI, 2.3.), as further specified under section III.A.2;
3. Spectral data (Annex VI, 2.3.5.), as further specified under section III.A.3;
4. Description of the analytical methods (Annex VI, 2.3.7.), as further specified under section III.A.4.

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated registration to ECHA by **8 December 2014**.

## III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein does not comply with the requirements of Article 10 of the REACH Regulation and Annex VI thereof. Consequently, the Registrant is requested to submit the information mentioned above that is needed to bring the registration into compliance with the relevant information requirements.

### A. Information in the technical dossier related to the identity of the substance

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

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

ECHA notes that the Registrant has not provided sufficient information to identify the substance, as required by Annex VI, Section 2.1 of the REACH Regulation. Based on the information included in Section 1.1 and 3.1 of the dossier, it is not possible to unambiguously establish the identity of the substance registered.

The Registrant identified the registered substance as of **Unknown** or **Variable** composition, **Complex** reaction products or **Biological** materials (UVCB). The naming of UVCB substances shall consist of two parts: the chemical name and the more detailed description of the manufacturing process, as indicated in chapter 4.3 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.2, March 2012) - referred to as "the Guidance" thereafter. According to the 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. ECHA observes that the Registrant did not provide sufficient information on the manufacturing process description to allow for an accurate and complete identification of the registered substance, as explained hereinafter.

More specifically, no manufacturing process description was provided in IUCLID section 1.1 and the description of the manufacturing process as reported in IUCLID section 3.1 does not sufficiently describe the identity of the starting materials, the ratio of the reactants and the relevant process parameters and steps.

The Registrant provided the chemical name "Benzenesulfonic acid, 4-C10-13-sec-alkyl derivs." for the registered substance and described in Section 3.1 of the IUCLID dossier the manufacturing process to consist of the synthesis of linear alkylbenzene (LAB) and sulphonation of the benzene ring (para position indicated). It is stated that "[REDACTED]

[REDACTED]". However, the Registrant did not specify further the exact identity, including the composition of the linear alkylbenzene effectively used in the process. As the composition of this reagent is one of the major factors determining the composition of the registered substance, compositional information of this starting material is a necessary element for its identification and therefore for the identification of the registered substance itself.

Furthermore, the chemical name provided in Section 1.1 and the description of the manufacturing process in Section 3.1 do not contain indications about the ratio of reactants and do not specify sufficiently the manufacturing process steps and parameters which are necessary to obtain the registered substance. Specification of the ratio of reactants and identification of any other steps and process parameters that may affect the substance composition is essential for the identification of the registered substance.

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

In line with the above observations and pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the missing information on the manufacturing process description. This information shall include:

- Information on the identity, and in particular the composition of the "linear alkylbenzene" starting material in terms of the concentration ranges of the groups of constituents presenting the same alkyl substituent carbon chain length (for example C10-alkyl benzenes, C11-alkyl benzenes, etc.), as well as information on the relative content of the individual isomers within a specific group of constituents (for example for C10-alkyl benzenes the distribution between 2, 3, 4, 5-phenyl C10 alkanes), and
- The identity of the sulfonating agent used, and the effect of using different sulfonating agents as the Registrant has indicated the use of "[REDACTED]" in section 3.1, and
- Ratio of reactants, and
- Specifications of all relevant process parameters, including temperatures and pressures, 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, and
- Information on the selectivity control of the sulfonation step towards specific alkylbenzene substitution with the sulfonic group.

If the substance covered by the registration is manufactured according to different manufacturing processes, including the use of different sources, then the detailed description of the manufacturing process required hereinabove shall be reported separately for each manufacturing process. A manufacturing process may be considered different when the processing steps and/or processing parameters are different.

The Registrant shall note that substances manufactured according to different manufacturing processes may indicate multiple substances and consequently the requirement for multiple registrations.

As for the reporting of the requested information, the more detailed description of the manufacturing process should be included in the description field in section 1.1 of the IUCLID dossier.

## 2. Composition of the substance (Annex VI, 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.

ECHA notes that the registration does not contain sufficient and appropriate information for establishing the composition of the registered UVCB substance and therefore its identity, as required under Annex VI, section 2.3. of the REACH Regulation.

In particular, the reported composition refers to groups of constituents defined according to the carbon chain length of the alkyl substituent (e.g. "4-[decan-(2 to 5)-yl] benzenesulfonic acid") for which the IUPAC names and structural formulas are in line with the identifiers for the registered substance, where the alkyl substituents are attached from non-terminal carbons. The typical, minimum and maximum concentration levels for each of the groups of constituents were provided as well. However, the EC and CAS identifiers given for these groups of constituents are specific for well-defined compounds with alkyl groups attached from the terminal carbon and therefore do not correspond with the IUPAC names and structural formulas provided for the groups of constituents, or with the identifiers used to describe the identity of the UVCB substance in section 1.1.

In addition, ECHA notes that the Registrant indicates broad concentration ranges of [REDACTED] for the group of constituents "4-[decan-(2 to 5)-yl] benzenesulfonic acid", [REDACTED] for "4-[undecan-(2 to 6)-yl] benzenesulfonic acid", [REDACTED] for "4-[dodecan-(2 to 6)-yl] benzenesulfonic acid" and [REDACTED] for "4-[tridecan-(2 to 7)-yl] benzenesulfonic acid", in IUCLID section 1.2, which is not justified by the manufacturing process description due to its lack of detail as has been explained under section III.A.1 hereinabove.

Furthermore, the information on the distribution of individual positional isomers for each group of constituents has also not been provided although the individual isomers, as known constituents, should be reported following section 4.3.1.1 of the Guidance. This information is important in order to understand the variability of the composition of the registered substance. In addition, all constituents present in the substance with a concentration of  $\geq 10$  %, as well as those relevant for the classification and/or PBT assessment cannot be reported as a group, but shall be identified and reported individually.

ECHA therefore concludes that the composition of the registered substance has not been sufficiently specified.

The Registrant is accordingly requested, pursuant to Article 41(1) and (3) of the REACH Regulation, to revise the information on the composition of the registered substance in order to establish a precise chemical representation of what the substance consists of. The consistent and representative identifiers for each group of constituents presenting the same alkyl substituent carbon chain length (EC and CAS identifiers shall be provided only if applicable) together with the information on the distribution of individual positional isomers

for each group of constituents shall be provided. Furthermore, all constituents present in the substance with a concentration of  $\geq 10\%$ , all other known constituents/groups of constituents in addition to the alkyl benzenesulfonic acids, as well as those constituents relevant for the classification and/or PBT assessment shall be identified and reported individually.

In addition, the Registrant is requested to amend the concentration range values for the different groups of constituents. The concentration range values must be representative for the registered substance as manufactured and it shall be clarified how the minimum and maximum values for each group of constituents were obtained (i.e. information on the batch selection, sampling procedure, the measured values, calculations used etc.). Without this information ECHA is not able to conclude on the representativeness of these values.

Where the Registrant covers different grades of the substance in the registration, the Registrant shall report separately the compositional information of each grade. This means that if the substance covered by the registration has two (or more) different compositions, then these must be presented separately. ECHA highlights that failure to report separately the compositional information of each grade of a substance may result in one or more grades not being covered by this registration.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: The Registrant shall indicate the composition of the registered substance in IUCLID Section 1.2. For each constituent required to be reported individually, the IUPAC name, CAS name and CAS number (if available), molecular and structural formula, as well as the minimum, maximum and typical concentration, 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.

The information on the concentration levels of individual positional isomers (i.e. 2, 3, 4, 5-phenyl C10 alkanes; 2, 3, 4, 5, 6 - phenyl C11 and C12 alkanes and 2, 3, 4, 5, 6, 7- phenyl C13 alkanes) present in the substance composition shall be specified in the "Remarks" field of each group of constituents.

Information on how to report several compositions in IUCLID is specified in paragraph 2.3, Q&A8 of the "Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH" (version: 2.0, July 2012), available on the ECHA website.

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

ECHA observes that the Registrant has not included sufficient spectral data required by Annex VI, Section 2.3.5. of the REACH Regulation for the identification of the registered substance.

More specifically, ECHA notes that the registration does not contain the Ultra-Violet (UV) and Nuclear Magnetic Resonance (NMR) or Mass Spectrum (MS) spectral data required according to Annex VI Section 2.3.5. of the REACH Regulation to support the identity of the registered substance.

ECHA regards this required information scientifically relevant for the registered substance for the following reasons:

- The substance absorbs in the UV range due to the presence of chromophores in the composition. A UV spectrum representing the absorption of these constituents in the UV range can therefore be recorded;
- NMR spectroscopic analyses such as a <sup>1</sup>H-NMR or a <sup>13</sup>C-NMR are powerful tools for structure characterisation and elucidation due to characteristic chemical shifts and spin-spin coupling which also reflects the relative abundance of individual atoms. As all reported constituents contain characteristic hydrogen and carbon atoms, NMR is an appropriate analytical method to characterise the substance.

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

Accordingly, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the missing UV and NMR spectra. Alternative to NMR, a mass spectrum including the corresponding interpretation of the fragmentation scheme can be provided.

The Registrant shall ensure that the description of the analytical methods used for the recording of the spectral 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.

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

#### 4. Description of the analytical methods (Annex VI, 2.3.7)

ECHA notes that the Registrant has not provided sufficient information on the analytical methods used to determine the composition of the registered substance, as required by Annex VI, Section 2.3.7. of the REACH Regulation.

More specifically, the dossier submitted by the Registrant contains a GC chromatogram (GC-MS analysis, attachment [REDACTED]), as required by Annex VI Section 2.3.6. Moreover, in the report of the analysis (attachment [REDACTED]) the Registrant states that [REDACTED]

[REDACTED]. However, the results indicated in the result table (attachment [REDACTED]) do not reflect in detail the peaks observed in the chromatogram. The assignments and peak areas of the chromatogram peaks of individual isomers present in the substance is missing from the table. Therefore it is not possible to verify the correspondance of the individual peaks (of the constitutional isomers) with the more generic results provided for the groups of constituents, or to conclude on the ratios of the individual isomers in the substance. In the absence of this information, the composition of the registered substance cannot be verified.

ECHA therefore concludes that the Registrant did not provide sufficient information on the description of the analytical methods used for quantification of the composition of the registered substance in terms of individual constituents present in the substance.

Accordingly, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to provide detailed description of the analytical method(s) used for identification and quantification of the registered substance including the constituents present. 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 chromatographic methods, 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. In addition, the Registrant shall ensure that the composition reported in Section 1.2 is in line with the information provided in Section 1.4, which shall be sufficient to identify and quantify the substance.

As for the reporting of the additional analytical data in the dossier, the information should be attached in Section 1.4 of the IUCLID Dossier.

#### IV. Information on right to appeal

An appeal may be brought against this decision to the Board of Appeal of ECHA under Article 51(8) of the REACH Regulation. Such an appeal shall be lodged within three months of receiving notification of this decision. Further information on the appeal procedure can be found on ECHA's internet page at <http://www.echa.europa.eu/regulations/appeals>. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.



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