EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004764-68-03/F Helsinki, 23 April 2015

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., EC No 287-494-3 (CAS No 85536-14-7), 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., EC No 287-494-3 (CAS No 85536-14-7), 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 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 30 October 2013.

On 19 December 2013 ECHA sent the draft decision to the Registrant and invited him to provide comments in accordance with Article 50(1) of the REACH Regulation on the draft decision.

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 by 7 April 2014, ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

II. Information required

A. 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 **30 July 2015.**

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 **U**nknown or **V**ariable composition, **C**omplex reaction products or **B**iological 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" thereinafter. 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 "[redacted]", followed by the reaction of obtained sulfur trioxide with a "[redacted]". However, the Registrant did not specify further the exact identity, including the composition, of the [redacted] 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 sufficient indications about the ratio of reactants and do not specify 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, in particular the composition of the "[redacted]" 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
- 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. "[redacted]"), along with the typical concentrations for each group of constituents. However, the Registrant did not provide information on the concentration ranges for any of these groups of constituents. In line with the chapter 4.3 of the Guidance, the Registrant should note that, for each constituent or group of constituents, the typical, minimum and maximum concentration levels shall be specified. In addition, all constituents present in the substance with a concentration of ≥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.

Furthermore, the Registrant states in the "Description" field of each group of constituents, that the entry covers different position isomers (e.g. [redacted]" etc.). Nevertheless, information on the distribution of individual positional isomers for each group of constituents has 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.

ECHA also notes that the composition information in section 1.2 is not consistent with the quantitative chemical analyses included in section 1.4 of the dossier, as further specified under section III.A.4.

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 information on the concentration ranges (minimum and maximum) for each carbon number (i.e. C10, C11, C12 and C13) 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 ≥10 %, as well as those relevant for the classification and/or PBT assessment shall be identified and reported individually.

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 as 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 Infra-Red (IR) 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;
- The IR spectrum displays characteristic vibration bands of covalent bonds in molecules present in the substance, including characteristic vibration bands from the chemical functionalities expected to be present in the composition;

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 IR spectra.

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 Registant did not utilise a direct analytical method for the quantification of the constituents as the quantification is based on the comparison of the distribution pattern of the different [redacted] in the starting material and the distribution pattern of the [redacted] in the final product. The Registrant states in the "Remarks" field of the GC-MS method in section 1.4 that the submitted gas chromatographic (GC-MS) experiment (attachment "[redacted]") "shows the mass-spectra of different isomers of the [redacted] used as raw material to obtain the [redacted]" and "Homolog/isomers distribution remain constant after [redacted] process and are identified by retention time". Nevertheless, no further explanation and data are provided to prove this statement and to explain, how the quantification has been performed.

Moreover,the dossier submitted by the Registrant contains GC-MS analysis results including a chromatogram of the "raw material" and a table with peak numbers, retention times peak height and peak areas (attachment "[redacted]"). However, the assignments of the chromatogram peaks to individual isomers present in the analysed substance are not included in the table. Furthermore, no GC-MS analysis results of the [redacted]—which could give information on the distribution of the positional isomers in the product—is presented in the dossier.

ECHA also notes, as indicated under section III.A.2, that the composition information included section 1.2 of the dossier is not consistent with the quantitative chemical analyses included in section 1.4 of the dossier. The Registrant submitted a description of methods used to determine the "[redacted]" content and the sulfuric acid content in the substance (attachment "[redacted]"). Results of these analysis are presented in the submitted Certificate of analysis (attachment "[redacted]"), however these constituents have not been included in the composition of the substance in section 1.2.

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.

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/group of constituents. 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 method descriptions 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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