Decision number: CCH-D-0000004631-79-03/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 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. Description of the analytical methods (Annex VI, 2.3.7), as further specified under section III.A.3.

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 **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 sulfonation of linear alkylbenzene "[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. In addition, no details of the starting material described as "[redacted]" are provided. The identity of starting materials are essential for the identification of a UVCB substance. Therefore, the identity of the starting material described as "[redacted]" should be provided as well.

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
- Exact identity of the starting material described as "[redacted]", 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"), along with the typical, minimum and maximum concentration levels for each of the groups of constituents. However, the Registrant did not provide information on the distribution of individual positional isomers for each group of constituents, 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 ≥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 information on the distribution of individual positional isomers for each group of constituents presenting the same alkyl substituent carbon chain length 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.

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. 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 for the identification and quantification 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 an HPLC chromatogram (HPLC-MS analysis, attachment "[redacted]"), as required by Annex VI Section 2.3.6. However, in the report of the analysis (attachment "[redacted]". However, ECHA observes that the Registrant did not provide any supporting analysis other than the attached HPLC-MS results to confirm the indicated amounts of the groups of constituents listed in Section 1.2. In addition, the results of the analysis did not provide any information on the distribution of individual positional isomers for each group of constituents which is required to be reported in Section 1.2 of the registration dossier. Therefore the results from an appropriate quantitative method that would confirm the concentrations of the constituents present in the substance has not been provided.

In the absence of this information, the composition of the registered substance cannot be verified.

Furthermore, the attachment "[redacted]" provided by the Registrant in section 1.4 of the IUCLID dossier includes spectral data required by Annex VI, Section 2.3.5, chromatographic data required by Annex VI, Section 2.3.6 and descriptions of analytical methods required by Annex VI, Section 2.3.7.

However, ECHA notes in general for the analytical information included in the above-mentioned attachment, that the information is not sufficient to allow the identity and composition of the registered substance to be verified, as the information is identical to the analytical information contained in a registration dossier submitted by a different legal entity. The analytical information is a fingerprint of a substance manufactured or imported by a specific registrant. Therefore, ECHA cannot establish whether the analytical information indeed relates to the substance covered by this registration or to the substance registered by the other legal entity.

Article 5 of the REACH Regulation requires legal entities to make sure that the substances they manufacture or place on the market are registered in accordance with Title II of the REACH Regulation. Based on Article 11(1) and 10(a)(ii) of the REACH Regulation, each Registrant is required to submit separately information on the identity of the substance he registers. Annex VI of the REACH Regulation provides that "the information given shall be sufficient to enable each substance to be identified". Analytical information generated on a substance that is not manufactured or imported by the Registrant cannot be used as evidence that would allow ECHA to verify the identity and composition of the registered substance.

Therefore, ECHA concludes that the analytical information provided by the Registrant cannot, in absence of further justification, be considered appropriate to verify the identity and composition of the registered substance.

In accordance with the above and pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is required to provide a description of the methods used to analyse the registered substance. The descriptions shall be given in such detail that the methods can be reproduced and shall therefore include detailed experimental protocols. The results of the analyses, generated on the substance as manufactured/imported by the Registrant, shall also be reported.

The spectral information shall be provided according to the requirements of Annex VI, Section 2.3.5. of the REACH Regulation.

Any (chromatographic) quantification method provided by the Registrant shall be appropriate to analyse the constituents of the substance required to be reported in the composition. The method shall be sufficient to identify and quantify the groups of constituents presenting the same alkyl substituent carbon chain length (for example C10-alkyl benzenes, C11-alkyl benzenes, etc.), as well as to provide information on the relative content of the individual isomers within a specific group of constituents.

For descriptions of chromatographic methods, the following are expected as a minimum; details of sample/standard preparation, column specification, and identity of carrier gas/eluent and detector type. The information shall also 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.

The Registrant shall remove from the registration dossier any analytical information that has not been generated on the substance as manufactured/imported by the Registrant. If any of the analytical information currently present in the registration dossier is relevant for the registered substance, a valid justification as to why this is the case shall be provided.

As for the reporting in the registration dossier, the information should be included 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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