ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114308067-56-01/F Helsinki, 31 August 2015

DECISION ON A COMPLIANCE CHECK OF A REGISTRATION PURSUANT TO ARTICLE 41(3) OF REGULATION (EC) NO 1907/2006

For Amines, tallow alkyl, dodecylbenzenesulfonates, EC No 268-766-0 (CAS No 68139-94-6), 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 Amines, tallow alkyl, dodecylbenzenesulfonates, EC No 268-766-0 (CAS No 68139-94-6), submitted by [redacted] (Registrant).

The scope of this compliance check decision 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 100 to 1000 tonnes per year. This decision does not take into account any updates after the date when the draft decision was notified to the Registrant under Article 50(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 9 February 2015.

On 29 April 2015 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision.

On 3 June 2015 ECHA received comments from the Registrant agreeing to ECHA's draft decision

On 23 July 2015 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

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, Section 2.1.)
2. Composition of the substance (Annex VI, Section 2.3.)
3. Description of the analytical methods (Annex VI, Section 2.3.7.)

B. Deadline for submitting the required information

Pursuant to Articles 41(4) and 22(2) of the REACH Regulation the Registrant shall submit to ECHA by **7 December 2015** an update of the registration dossier containing the information required by this decision.

III. Statement of reasons

Pursuant to Article 41(3) of the REACH Regulation, ECHA may require the Registrant to submit any information 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, Section 2.1)

"Name or other identifier of the substance" is an information requirement as laid down in Annex VI, Section 2.1. of the REACH Regulation. The name and other identifiers are used to identify the substance in an unambiguous manner and are therefore fundamental for substance identification. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the Registrant identified the registered substance as of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). In line with the Guidance for identification and naming of substances under REACH and CLP (Version: 1.3, February 2014) - referred to as "the Guidance" thereinafter, the naming of UVCB substances shall consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process.

ECHA observes that the Registrant provided a chemical name for the registered substance which corresponds to "Amines, tallow alkyl, dodecylbenzenesulfonates". However, ECHA underlines that the chemical name of the registered substance is not in line with the information obtained from the analytical data attached to IUCLID section 1.4 and used to identify the registered substance.

Specifically, according to the results of the liquid-chromatography-mass spectrometry (LC-MS) analysis, the estimated alkyl chain length distribution of the alkyl benzene sulphonate derivatives ranges from C10 to C13 (most abundant alkyl chain lengths) while the estimated alkyl chain distribution of the amine derivatives ranges from C14 to C18 (most abundant alkyl chain lengths). Additionally the LC-MS analysis indicates the presence of mono and di-alkyl benzene sulphonate species. Moreover, the generic tertiary amine structure provided in IUCLID Section 1.2 as well as in the analytical report, suggests that alkyl chains attached to nitrogen do not originate only from tallow, as there is also a methyl substituent attached to the amine nitrogen.

The provided chemical name, however, indicates the presence of an alkyl chain length for the alkyl benzene sulphonates corresponding to C12 and it does not reflect the presence of mono- and di-alkylbenzene sulphonate species nor gives any information on the type of amines (primary, secondary or tertiary; substituent not originating from tallow, i.e. methyl group).

ECHA concludes that the information provided on the chemical name of the registered substance is inconsistent with the information provided in IUCLID section 1.4. For this reason, the identity of the registered substance cannot be established.

Furthermore, ECHA observes that the description of the manufacturing process was not reported in section 1.1 of the registration dossier.

Accordingly, the Registrant is requested to clarify the information provided on the registered substance in relation to its chemical name. This shall include clarification on:

- The identity of the alkyl benzene sulphonate moiety in terms of alkyl chain length, possible branching and/or unsaturation of the alkyl chain;
- The content of mono- and di-alkyl benzene derivatives;
- The position of the alkyl substituent on the benzene sulphonate ring;
- The identity of the tertiary amines including information on their source, alkyl chain lengths, possible branching and unsaturation of the alkyl chains. It needs to be clarified by the Registrant whether tallow or tallow alkyl precursors were subject to any chemical modification such as hydrogenation.

Additionally, the description of the manufacturing process shall be sufficiently detailed to allow ECHA to verify the starting materials used and to verify how any other steps and process parameters may affect the substance composition and therefore its identity. It shall include, as appropriate:

- Information on the identity, and in particular the composition, of the starting materials. The description shall also include information on the exact identity and concentrations of the individual constituents/groups of constituents of the starting materials;
- Information on any chemical modification of the starting materials, specifically tallow precursors of tallow alkyl amines. Tallow normally contains approximately ■ % (w/w) of unsaturated fatty acids, while ECHA observes that the results of spectral analyses do not show significant presence of unsaturated species in the registered substance;
- Specification of the manufacturing process parameters (e.g. temperature, pressure, reaction time);
- Specification of the ratio of reactants;

- Furthermore, the Registrant shall provide information on any other relevant process steps and parameters including purification step(s) (if any) that are required for identifying the substance and may affect the substance composition.

The Registrant shall note that if the substance covered by the present 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.

Regarding how to report the requested information in the IUCLID dossier, the following applies as appropriate:

- The substance shall be named based on:
  - Alkyl amines moiety in terms of the source descriptor describing the origin of the animal fat used to manufacture the amines, any chemical modification of the starting materials (e.g. hydrogenation of tallow) and alkyl amines structure (primary, secondary or tertiary amines) including the alkyl descriptor (e.g. di-tallow alkyl methylamines).
  - The alkyl chain distribution of the benzene sulphonates moiety. The most abundant alkyl chain lengths that compose at least [redacted] % of the carbon number range need to be included in the name.
  - The position of the alkyl substituents on the benzene sulphonate rings.
- The revised name shall be reported in the IUPAC name field in IUCLID section 1.1.
- The description of the manufacturing process shall be included in the description of the substance field in section 1.1.
- The appropriate CAS entry shall be included in the "CAS information" field, if available. Where the current CAS entry (i.e. 68139-94-6) does not identify the registered substance, it should be reported under the "Related CAS information" field in IUCLID section 1.1.
  Similarly, where the current EC number does not correctly identify the registered substance, it will need to be revised. For technical reasons the Registrant is requested at this stage, not to remove or revise the EC entry in the updated dossier. As this registration is linked to this EC entry in REACH-IT, the IT system will not accept the updated dossier as an update when the EC entry has changed. The Registrant shall instead include the following in the "Remarks field" of the reference substance: "*This EC entry is not appropriate to identify the registered substance. This identifier cannot be modified in the present registration at this stage for technical reasons.*"

Further technical information is available in paragraph 2.1 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.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: correct name and other identifier of the registered substance as specifically explained above. The Registrant shall ensure that the information is consistent throughout the dossier.

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

"Composition of the substance" is an information requirement as laid down in Annex VI, Section 2.3. of the REACH Regulation. 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. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the Registrant has not included sufficient information on the composition of the substance to enable the identity of the registered substance to be verified, as required under Annex VI, Section 2.3. of the REACH Regulation.

More specifically, ECHA observes that the Registrant has reported in IUCLID Section 1.2 two constituents: "*Teriary amines/Generic group covering tertiary amine*" in concentration range between [redacted] % (w/w) and "*Alkyl benzene sulphonate/Generic group covering Dimer to Mono Alkyl benzene sulphonate*" in concentration range between [redacted] % (w/w) without providing further information on their molecular and structural formula, beside generic structures.

Additionally, ECHA notes that the Registrant included the results of a liquid-chromatography-mass spectrometry (LC-MS) analysis in IUCLID section 1.4 which provides an estimation of the alkyl chain length distribution of the alkyl benzene sulphonate species (C10 to C13) including a content of mono and di-alkyl benzene sulphonate derivatives present ([redacted] and [redacted] %, respectively) as well as an estimation of the alkyl chain length distribution of the tallow alkyl methylamine species (C14 to C18).

Consequently ECHA underlines that the compositional information reported in IUCLID section 1.2 is not sufficiently detailed neither it does adequately reflects the results of the LC-MS analysis attached to IUCLID section 1.4.

According to section 4.3. of the Guidance, for UVCB substances such as the registered substance, the Registrant shall note that the following applies:

- All constituents present in the substance with a concentration of ≥ 10 % shall be identified and reported individually;
- All known constituents and constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually; and
- Unknown constituents shall be identified as far as possible 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. This information must also allow ECHA to verify that the composition is consistent with the chemical name reported for the registered substance.

For each constituent or group of constituents, the typical, minimum and maximum concentration levels shall be specified.

The Registrant is accordingly required to revise the composition by providing the missing structural information which is suitable and necessary to allow ECHA to establish and verify the composition and the name of the registered substance. The Registrant shall report separately the constituents or group of constituents representing "dimers" and "monomers" of the alkylbenzene sulphonate derivatives.

Regarding how to report the information on the composition of the registered substance in IUCLID, the following applies: the Registrant shall report the composition 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.

Further technical details on how to report the composition of UVCB substances in IUCLID are available in paragraphs 2.1 and 2.2.2 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).

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: all identified constituents and impurities, with their typical concentrations and concentration ranges. The Registrant shall ensure that the information is consistent throughout the dossier.

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

"Description of the analytical methods" is an information requirement as laid down in Annex VI, Section 2.3.7. of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA observes that the Registrant did not provide sufficient and appropriate description of the analytical methods used for the identification and quantification of the constituents required to be reported in the composition of the registered substance, as requested according to Annex VI section 2.3.7.

Specifically, the Registrants has provided a full set of analytical data (elemental analysis, IR, UV, NMR and LC-MS) in IUCLID section 1.4 and used the liquid-chromatography-mass spectrometry (LC-MS) analysis to identify the main classes of constituents. Nevertheless, the Registrant claimed that *"it is not possible to give a meaningful estimation of each of these three compound classes"*. The Registrant instead described the approach followed to estimate the alkyl chain length distribution of the alkyl benzene sulphonate derivatives, the content of the mono-alkyl and di-alkyl benzene sulphonate derivatives and the alkyl chain length distribution of tallow alkyl methylamine derivatives.

ECHA underlines that it is not clear whether the composition of the registered substance was derived based on quantitative or semi-quantitative method. The analytical methods included in the dossier may not be sufficient to provide detailed information on the composition of the registered substance and its required subdivision into groups of constituents. As underlined already in section III.2 above, the Registrant shall describe separately the group of constituents "mono-alkylbenzene sulphonates", "di-alkylbenzene sulphonates" and "tertiary amines" and include in the dossier a quantitative method to identify and quantify all the groups of constituents.

ECHA therefore concludes that the description of the analytical methods used for the quantification of the constituents and the results thereof required to be reported is not sufficient.

Consequently, the Registrant shall provide a description of the analytical method(s), or the appropriate bibliographical references, used to identify and quantify the registered substance, including its composition. This information shall be sufficient to enable the substance identified in IUCLID section 1.1 and all constituents reported in IUCLID section 1.2 to be verified as revised based on requests in section III.1-2 above.The information shall be sufficient for the method to be reproduced and shall therefore include details of the experimental protocol followed, the calculation used and the result obtained. The information regarding the quantitative methods should be in such detail that all steps and calculations can be followed. The Registrant shall ensure that the composition reported in the dossier is consistent with the analytical results obtained.

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

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: correct description of the methods used to identify and quantify the registered substance as specifically explained above. The Registrant shall ensure that the information is consistent throughout the 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.

Authorised[1] by Claudio Carlon, Head of Unit, 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.