ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004092-83-02/F Helsinki, 13 December 2013

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

For Fatty acids, C14-18 and C16-18-unsatd., mixed esters with neopentyl glycol and trimethylolpropane, CAS No 85186-92-1 (EC No 286-078-9), 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 dossier for Fatty acids, C14-18 and C16-18-unsatd., mixed esters with neopentyl glycol and trimethylolpropane, CAS No 85186-92-1 (EC No 286-078-9) submitted by [redacted] (Registrant).

This decision is based on the registration dossier 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 5 September 2013, 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. The scope of this compliance check is limited to the standard information requirements of Annex VI, Section 2 of the REACH Regulation.

The compliance check was initiated on 29 March 2012.

On 21 August 2012 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision. That draft decision was based on submission number [redacted].

On 19 September 2012 the Registrant provided comments on the draft decision to ECHA.

On 07 January 2013 the Registrant updated his registration dossier (submission number [redacted]).

On 04 March 2013 the Registrant updated his registration dossier (submission number [redacted]).

On 25 March 2013 the Registrant updated his registration dossier (submission number [redacted]).

ECHA considered the Registrant's comments and the updates. Based on the comments and the updated dossier, Section II of the draft decision was amended and the Statement of Reasons (Section III) was modified accordingly.

On 5 September 2013 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 to amend the draft decision within 30 days of the receipt of the notification.

Subsequently, Competent Authorities of the Member States did not propose amendments to the draft decision and ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

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

II. Information required

Pursuant to Articles 41(1)(a), 41(3) and 10(a)(ii) as well as Annex VI, section 2 of the REACH Regulation the Registrant shall submit for the registered substance:

a. Name or other identifier of the substance (Annex VI, 2.1.), as specified under section III.(a) below;
b. Composition (Annex VI, 2.3.), as specified under section III.(b) below.

Taking into consideration the data currently available in the dossier, ECHA considers the following. Section III below specifies in detail all the information that ECHA considers appropriate in order to identify any substance of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). UVCB substances cannot be sufficiently identified by their chemical composition, because the number of constituents is relatively large; and/or the composition is, to a significant part, unknown; and/or the variability of composition is relatively large or poorly predictable. As a consequence, UVCB substances require other types of information for their identification, in addition to what is known about their chemical composition.

As a result, ECHA cannot be in a position, before receiving suitable information, to determine precisely the other types of information that is actually required to identify a specific UVCB substance. Only the Registrant of that UVCB substance knows the details of its identity. Based on this knowledge, he may consider that some of the information requested by ECHA is not suitable and necessary in order to identify the substance. Nevertheless, in this case it is the Registrant's exclusive responsibility 1) to ensure that ECHA is in a position to identify precisely the substance and 2) to justify the reasons for which some information requested may have been omitted.

Therefore, if the Registrant eventually decides to submit only part of the detailed information specified in Section III and if the submitted information does not enable ECHA to establish and verify the identity of the substance actually covered by the dossier, the registration will not be considered valid.

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated IUCLID dossier to ECHA by **13 March 2014**.

III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein, submitted by the Registrant for registration of the above mentioned substance for the purpose of registration within the applicable tonnage band of 100 to 1000 tonnes per year in accordance with Article 6 of the REACH Regulation, does not comply with the requirements of Articles 10 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.

ECHA wishes to stress that the information currently contained in the dossier which the present decision does not require to remove or modify is considered as necessary for the determination of the identity of the substance. Such information shall therefore not be removed or modified by the Registrant. In the absence of valid justification, any change made by the Registrant to such information will not be taken into consideration by ECHA and will be considered as a deliberate obstruction to the determination of the identity of the substance.

Pursuant to Article 10(a)(ii) and Annex VI, section 2 of the REACH Regulation, the technical dossier of the registration shall include information on the identity of the substance. Annex VI, section 2 lists information requirements that shall be sufficient to identify the registered substance.

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

ECHA notes that the Registrant identified the registered substance as of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). 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: 1.2, March 2012) - referred to as "the Guidance" thereinafter. Other identifiers, including any CAS number (if available) and EC number (if available and appropriate) corresponding to the substance, shall also be reported. ECHA observes that the Registrant did not provide sufficient and appropriate information on the naming of the registered substance (as explained under point (i) thereinafter), including also the assigned CAS identifier (as indicated in point (ii) thereinafter).

(i) A chemical name representative of the registered substance

The chemical name reported in the dossier originally submitted indicated that the registered substance corresponded to esters of "Fatty acids, C14-18 and C16-18-unsatd.". ECHA considered that the name "Fatty acids, C14-18 and C16-18-unsatd.", which according to the Guidance represents fatty acids with both even- and odd-carbon numbers, was not representative of the fatty acids actually used in the manufacturing process. The [redacted] origin of these fatty acids, as specified in the manufacturing process, indeed indicated that these fatty acids were to be represented by structures of even-carbon numbers. In addition, the chemical name originally specified in the registration dossier did not make reference to the level of esterification of the neopentyl glycol and trimethylolpropane in the substance. For these reasons, ECHA considered that the chemical name assigned to the

registered substance in the dossier initially submitted was inappropriate for its unambiguous identification. ECHA thus requested in its draft decision the Registrant to revise the chemical name assigned to the registered substance.

ECHA notes that the registrant revised, in a registration update following the notification of the draft decision (thereinafter the "update dossier"), the chemical name assigned to the registered substance to "Fatty acids, C16, C18 and C18unsatd., mixed esters with neopentyl glycol and trimethylolpropane". ECHA understands that the fatty acids used for the manufacturing of the registered substance refer, according to this chemical name, to a starting material comprising, in line with the Guidance, linear saturated carboxylic acids with chain lengths C16 and C18 as well as linear unsaturated fatty acids with chain length C18.

However, ECHA also observes that the Registrant specified, in the Description field in IUCLID section 1.1 and in IUCLID section 3.1 of the update dossier, the compositional profile of the fatty acids used for the manufacturing process description. According to this composition, the linear saturated carboxylic acid with chain length C18, which is quoted in the chemical name of the registered substance, is present at a concentration of [redacted]%. However, the linear unsaturated carboxylic acid with chain length C16, which is not quoted in the chemical name of the registered substance, is present at a higher concentration ([redacted]%).

ECHA therefore concludes that the chemical name "Fatty acids, C16, 18 and C18-unsatd." is not a representative descriptor of the fatty acids involved in the manufacturing of the registered substance under REACH.

In addition, the chemical name of the registered substance specified in the update dossier does not make reference to the level of esterification of the neopentyl glycol and trimethylolpropane in the substance, although this issue was already pointed out in the draft decision.

ECHA therefore concludes that the chemical name assigned to the registered substance is not appropriate for its unambiguous identification.

The Registrant is accordingly required to revise the chemical name assigned to the registered substance, as specified under the first bullet point of sub-section (iii) below.

(ii) <u>The CAS information</u>

The CAS name corresponding to the CAS entry with CAS number 85186-92-1 assigned to the substance in the dossier initially submitted is "Fatty acids, C14-18 and C16-18-unsatd., mixed esters with neopentyl glycol and trimethylolpropane". In line with the abovementioned observations on the chemical name assigned to the registered substance, such CAS entry does not specifically correspond to the registered substance. ECHA thus requested in its draft decision the Registrant to delete from the "CAS information" header in section 1.1 of the IUCLID dossier the CAS entry with CAS number 85186-92-1. ECHA also indicated that the Registrant could nevertheless report this CAS entry under the "Related CAS information" header in IUCLID section 1.1.

ECHA observes that the Registrant reported, under the "Related CAS information" header in IUCLID section 1.1 of the update dossier, the CAS entry with CAS number 85186-92-1. ECHA also observes that the Registrant clarified, in the Remarks field of the reference substance in IUCLID section 1.1 of the update dossier, that the EC entry 286-078-9 currently assigned to the substance (which is itself linked to the CAS number 85186-92-1) does not specifically corresponds to the registered substance. The Registrant nevertheless maintained the CAS entry with CAS number 85186-92-1 under the "CAS information" header. ECHA underlines that it is a prerequisite that the CAS number reported in the dossier matches the substance registered under REACH, i.e. it does not contradict the substance identity provided for by the naming of the registered substance.

ECHA therefore concludes that the Registrant did not address this issue already specified in the draft decision.

The Registrant is thus required to revise the CAS information for the registered substance, as specified under the second bullet point of sub-section (iii) below.

(iii) The information required from the Registrant

- A chemical name representative of the registered substance must be provided

Based on the observation set out in sub-section (i) above, the Registrant is accordingly requested to revise the chemical name assigned to the registered substance.

Regarding the designation of the fatty acids starting material in the chemical name of the registered substance, ECHA points out that constructing the chemical name on the basis of:

- the main fatty acids (i.e. those linear fatty acids which individually present an upper concentration level ≥10% (w/w) in the starting material); and
- the groups of unsaturated fatty acids presenting the same carbon number and an upper concentration level ≥10% (w/w) in the starting material

is appropriate provided that they altogether compose at least 80 % (w/w) of the substance. If this condition is not met, all fatty acid constituents in the starting material, as identified by their carbon number and alkyl chain type (e.g. saturated, unsaturated) shall be taken into account for the naming of that starting material. Where the starting material is composed of one specific fatty acid at a concentration level of ≥80% (w/w), this starting material shall be designated, in the chemical name of the registered substance, by the chemical name of that fatty acid.

Furthermore, regarding the information on the level of esterification in the chemical name, reference to the main group(s) of ester constituents presenting the same degree of esterification (i.e. monoesters and/or diesters with neopentyl glycol and/or the monoesters, diesters and/or triesters with trimethylolpropane) shall be made in the chemical name of the registered substance. Such main group is the group present at a concentration level of ≥80% (w/w) in the registered substance. If such group does not exist, all the groups present at a concentration of ≥10% (w/w) designate the main group(s) that shall be referred to in the chemical name.

- The CAS information must be revised

  Based on the observation set out in sub-section (ii) above, the Registrant shall delete from the "CAS information" header in IUCLID section 1.1 of the update dossier the CAS information currently assigned to the substance. The Registrant shall provide instead any available CAS information specifically corresponding to the substance.

ECHA recognises that the Registrant may cover different grades of the same substance in a registration based on different sources and/or different manufacturing processes. In these cases, the Registrant shall provide the required information on the sources, manufacturing processes and constituents of each grade. ECHA underlines that the reporting of a generic process description covering the manufacturing of different grades may prevent ECHA from concluding that the manufacturing of other substances is not covered by that description. In addition, ECHA highlights that grades for which a description would not be provided may eventually not be considered as being covered by the registration.

More generally, the Registrant should note that substances manufactured according to different manufacturing processes may indicate multiple substances and may, consequently, require multiple registrations. ECHA has established processes, subject to certain conditions, enabling registrants to adapt an existing registration, while maintaining the regulatory rights already conferred to the substance concerned. Should the Registrant consider that his dossier actually concerns several substances, he is thus encouraged to contact ECHA for a possible adaptation of the registration.

As for the reporting of the information in IUCLID, the chemical name, manufacturing process description and any available CAS entry for the substance should be specified in the "IUPAC name" field, "Description" field and under the "CAS information" header in IUCLID section 1.1, respectively. The CAS entry with CAS number 85186-92-1 can be kept under the "Related CAS information" header in IUCLID section 1.1.

The Registrant shall ensure that the correct identifiers are used throughout the registration whenever reference to the specific substance which is the subject of this registration is made.

(b) Composition (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 corner stone of all the REACH obligations.

The Registrant did not report, in section 1.2 of the IUCLID dossier initially submitted, any of the constituents or groups of constituents required to be identified and quantified in the composition of the registered substance, as required under Annex VI, section 2.3. of the REACH Regulation. ECHA thus requested, in its draft decision, the Registrant to provide detailed compositional information of the registered substance.

ECHA notes that the Registrant provided, in the update dossier, detailed compositional information on the registered substance. However, the 3rd, 5th and 7th listed constituents reported in IUCLID section 1.2 of the update dossier have not been correctly specified as they refer to derivatives of C17 unsaturated fatty acids while the analytical data would indicate that the C17 unsaturated fatty acid building block should in fact correspond to C18 unsaturated fatty acid block. Furthermore, discrepancies exist on the stereochemistry of the unsaturation in at least the linear unsaturated C18 fatty acid moiety of the ester constituents. At least for this block, the Registrant inconsistently refers to the presence of only one of the possible isomers (either E or Z) or does not provide any information at all on the stereochemistry.

ECHA therefore concludes that the reported composition of the registered substance in the update dossier includes inappropriate information.

The Registrant is accordingly required to revise the compositional information of the registered substance by addressing the abovementioned discrepancies.

According to chapter 4.3 of the Guidance, the Registrant is reminded that, for UVCB substances 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 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.
  For the substance which is the subject of this registration, the reporting of the unknown ester functionalised constituents according to groups presenting the same polyol building block, the same level of esterification and the same combination of fatty acid building blocks according to the carbon numbers is necessary for this aforementioned purpose. For each group of constituents, information on the relative content between saturated and unsaturated fatty acid blocks of the same carbon number shall also be specified.

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

Where the Registrant covers different grades of the substance in a registration based on different constituents, the Registrant shall report separately the source, manufacturing process and the compositional information of each grade. ECHA underlines that the reporting of the composition of different grades under one generic composition may prevent ECHA from verifying that compositions referring to other substances are not covered by this registration. In addition, ECHA highlights that grades for which an individual composition would not be provided may eventually not be considered being covered by the registration.

More generally, the Registrant should note that multiple compositions may indicate multiple substances and may, consequently, require multiple registrations. ECHA has established processes, subject to certain conditions, enabling registrants to adapt an existing registration, while maintaining the regulatory rights already conferred to the substance concerned. Should the Registrant consider that his dossier actually concerns several substances, he is thus encouraged to contact ECHA for a possible adaptation of the registration.

Regarding how to report the composition in IUCLID, the following applies: The Registrant shall indicate each 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, 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. Information on the relative content between saturated and unsaturated fatty acid blocks of the same carbon number should be specified in the "Remarks" field of the repeatable block for that group.

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) on the ECHA website. Information on how to report several compositions in IUCLID is specified in paragraph 2.3, Q&A8 of that manual.

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/web/guest/regulations/appeals. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

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