ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004080-88-02/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, C16-18, esters with pentaerythritol, CAS No 85116-93-4 (EC No 285-547-5), 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, C16-18, esters with pentaerythritol, CAS No 85116-93-4 (EC No 285-547-5) submitted by [redacted] (Registrant).

This decision is based on the registration dossier 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 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 07 August 2012.

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

On 18 September 2012 the Registrant provided comments on the draft decision to ECHA.

On 14 December 2012 the Registrant updated his registration dossier (submission number [redacted]).

On 15 August 2013 the Registrant updated his registration dossier (submission number [redacted]).

ECHA considered the Registrant's comments and the updated dossier. 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 of the substance (Annex VI, 2.3.), as specified under section III.(b) below;
c. Description of the analytical methods or the appropriate bibliographical references for the identification of the substance (Annex VI, 2.3.7.) as specified under section III.(c) 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 that 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 1000 tonnes or more 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 points (i) and (iii) thereinafter), including also the assigned CAS identifier (as indicated in point (ii) thereinafter).

(i) A chemical name representative of the registered substance

The Registrant did not originally specify the chemical name of the UVCB substance which should be provided in the "IUPAC name" field, as indicated in chapter 8.2.4 of the Guidance. ECHA thus requested in its draft decision the Registrant to provide the missing chemical name. ECHA also requested the Registrant to ensure that the chemical name to be assigned to the registered substance designates the fatty acids and defines the level of esterification in accordance with specific principles specified in the draft decision.

ECHA notes that the Registrant assigned, in a registration update following the notification of the draft decision (thereinafter the "update dossier"), a chemical name indicating that the registered substance refers to esters of "fatty acids, C16-18, (even numbered)" with pentaerythritol. However, this chemical name does not specify any information on the degree of esterification of the registered substance.

ECHA therefore concludes that the Registrant did not address the incompliance on the chemical name of the registered substance, which was requested in the draft decision.

The Registrant is still requested to revise the CAS information for the registered substance, as specified under the first bullet point of sub-section (iv) below.

(ii) The CAS information

The chemical name associated with the CAS number 85116-93-4 assigned to the registered substance in the dossier initially submitted indicated that the registered substance corresponds to esters of C16-18 fatty acids with pentaerythritol. ECHA understands from this information that such fatty acids refer at least to a starting material comprising the linear carboxylic acids with chain lengths C16, C17 and C18. However, ECHA noted that the compositional information reported by the Registrant in IUCLID section 1.2 indicated that the registered substance only consisted of derivatives of fatty acids presenting even carbon numbers, including C16 and C18. The absence of C17 fatty acid derivatives implied that the CAS entry with CAS number did 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 85116-93-4. 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 85116-93-4. 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 285-547-5 currently assigned to the substance (which is itself linked to the CAS number 85116-93-4) does not specifically correspond to the registered substance. The Registrant nevertheless maintained the CAS entry with CAS number 85116-93-4 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. This information shall not contradict with the substance identity provided for by the naming of the registered substance. ECHA therefore concludes that the Registrant did not address the request specified in the draft decision.

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

(iii) The manufacturing process

The ratio of reactants used and specifications of any other manufacturing process parameters determining the degree of completion of the esterification reaction (such as the acid and saponification values) were not indicated in the original dossier. ECHA pointed out in the draft decision that such parameters are essential elements of the manufacturing process as they determine the composition of the registered substance and requested the Registrant to include this information in the manufacturing process description.

ECHA notes that the Registrant has specified, in IUCLID section 1.1 of the update dossier that the degree of esterification is determined by the stoichiometry. The Registrant also reported, in IUCLID section 3.1 of the update dossier, alternative ratio of reactants and process conditions (in terms of temperature and pressure) for the manufacturing of compositions with different degrees of esterification. These compositions are referred to by the Registrant as "*di-ester batch*", "*tri-ester batch*" and "*tetra-ester batch*". In addition, the Registrant provided analytical information for compositions designated as "*di-ester rich grade* ", "*tri-ester rich grade*" and "*tetra-ester heavy grade*". ECHA therefore concludes that the dossier update currently makes reference to different grades.

The typical overall concentration ranges mentioned by the Registrant for the mono-, di-, tri- and tetra-esters in IUCLID section 1.1 ("*mono* [redacted], *di* [redacted], *tri* [redacted], *and tetra* [redacted]") indicate that the composition of these different grades referred to in the dossier update vary significantly from one grade to another. For example, the reported typical concentration range for the di-esters indicate that one of the grades includes insignificant concentration level of di-esters while other grade(s) predominantly consist of such di-ester constituents. This is also consistent with the differences observed between the chromatographic fingerprints from derivatised samples included in the registration update. The sample manufactured from a lower ratio of pentaerythritol to fatty acids shows a relative integral area of the derivatised di-ester of [redacted]%. In contrast, the sample manufactured from a "higher" ratio of pentaerythritol to fatty acids shows a relative integral area of the derivatised di-ester of [redacted]% of the total peak area.

It follows from the above that the manufacturing of the different grades mentioned in the update dossier involves significant changes of the process. This would be likely to lead to different substances that should be registered separately, as explained in Chapter 4.3 of the Guidance.

However, the Registrant did not report individually the process description for the grade(s) covered by the registration. ECHA therefore cannot associate the registration to any of the grades mentioned in the dossier or any individual substance.

ECHA therefore concludes that the manufacturing process has not been provided to a sufficient and appropriate level of detail for the identification of the registered UVCB substance.

The Registrant is still requested to provide the specific ratio of reactants used and specifications of any other manufacturing process parameters determining the degree of completion of the esterification reaction for the manufacturing of grade covered by the registration, as specified under the third bullet point of sub-section (iv) below.

(iv) 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 required to revise the chemical name assigned to the registered substance so as to reflect its degree of esterification. For this purpose, reference to the main group(s) of ester constituents presenting the same degree of esterification (i.e. monoesters, diesters, triesters and/or tetraesters with pentaerythritol) shall be specified 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) to be referred to in the chemical name.

ECHA wishes to stress that the level of esterification to be specified in the chemical name shall be representative of each individual grade of the same substance. The level of esterification shall not reflect the overall variations observed between different grades corresponding to different substances.

- 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.

- Further detail on the manufacturing process must be provided.

Based on the observation set out in sub-section (iii) above, the Registrant is required to submit the following information on the manufacturing process description for the grade covered by this registration:

- The exact ratio of reactants, and
- Specifications of the process parameters determining the degree of completion of the esterification, such as the acid and saponification values.

ECHA has underlined that the information provided by the Registrant in the updated dossier indicates that several grades are referred to in the dossier update. Where the registration covers more than one grade of the substance subject to this registration, the Registrant shall provide the required information on the source, 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. The Registrant shall remove from the dossier any information related to any grade of

another substance than the substance covered by this registration. 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 consequently the requirement for 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 and the description should be specified in the "IUPAC name" and "Description" fields in IUCLID section 1.1, respectively. Any available CAS information should be reported under the CAS information header of the reference substance in IUCLID section 1.1. The CAS entry with CAS number 85116-93-4 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.

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

More specifically, ECHA noted that the Registrant did not provide, in the dossier initially submitted, any information on the typical concentration levels of the constituents reported in the composition. In addition the dossier did not include any detail of the lower concentration levels of the unreacted fatty acids as well as the monoesters, diesters, triesters and tetraesters identified by the registrant. Without this information, ECHA could not conclude on the variability of the composition covered by the registration. ECHA thus requested in its draft decision the Registrant to specify the missing concentration values in the composition reported in IUCLID section 1.2. ECHA also requested the Registrant to report separately the composition of each grade of the same substance covered by the registration.

ECHA notes that the Registrant did not revise, in IUCLID section 1.2 of the update dossier, the compositional information originally included in the initial dossier. The Registrant instead mentioned, in the Description field in IUCLID section 1.1 of the update dossier, a "*typical concentration range*" the mono-, di-, tri- and tetra-esters in IUCLID section 1.1 ("*mono* [redacted] *di* [redacted], *tri* [redacted] *and tetra* [redacted]"). However, as already underlined in section III(a)(iii) of this decision, this information cannot be used to conclude on the variability of any individual grade as it would represent the variability in the concentration values between different grades. Furthermore the manufacturing of the different grades mentioned in the dossier involves significant changes of the process, which would be likely to lead to different substances that should be registered separately.

ECHA therefore concludes that the Registrant did not provide the compositional information on the registered substance requested in the draft decision. The compositional information currently present in the dossier is still not provided to the required level of detail.

The Registrant is therefore required to submit the following compositional information, in accordance to chapter 4.3 of the Guidance for the specific grade covered by the registration:

- 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.

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

In addition, as already explained in section III.(a) of this decision, ECHA considers that the Registrant makes reference to different grades in the update dossier. Where the Registrant covers different grades of the same substance in a registration, 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. The registrant shall remove from the dossier any compositional information related to a grade of another substance than the substance 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 consequently the requirement for 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 registration.

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.

(c) The description of the analytical methods (Annex VI, 2.3.7.)

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

ECHA notes that the Registrant provided, in the initially submitted dossier, a report from the gas chromatographic (GC) analysis of a sample that has been derivatised by a silylation reagent. The percentage of the derivatised constituents had also been reported (as integral area percentage) in the table. However, the analytical report did not provide details of the protocol followed to translate the results from the chromatographic analysis into concentration values of the constituents present in the derivatised sample and of the constituents present in the composition of the registered substance itself. In addition, the Registrant did not specify any description of the analytical method used for the identification and quantification of residual fatty acids as well as the monoesters and diesters in the substance. ECHA therefore requested the Registrant to provide a full description of the analytical methods used for the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance.

ECHA notes that the Registrant complemented, in the update dossier, the GC analytical report with an additional page specifying the relative integral area of residual fatty acids, pentaerythritol diesters and C17 tetraesters. However, the protocol followed to translate the results from the chromatographic analysis into concentration values of the constituents present in the derivatised sample and of the constituents present in the composition of the registered substance is still missing. In addition, the Registrant included a second GC report for another sample that has also been derivatised by a silylation reagent. This report provides the same level of detail on the description of the method used as in the first GC report.

In addition, the result from these two report indicate significant differences in the integral areas, as already illustrated in section III.(a)(iii) of this decision. These two GC reports included in the update dossier refer to the analysis of samples of different substances that should be registered separately, as explained in section III.(a)(iii) of this decision.

ECHA therefore concludes that the Registrant did not address the incompliance on the description of the analytical methods, which was specified the draft decision.

The Registrant is still required to provide a description of the analytical methods used for the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance. 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. The Registrant shall also remove from the dossier any analytical data related to a grade of another substance than the substance covered by this registration.

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

The Registrant shall ensure that any composition reported in the dossier is consistent with the analytical results obtained.

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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