

Decision number: CCH-D-0000004103-88-02/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, C14-18 and C16-18 unsatd., triesters with trimethylolpropane, CAS No 68002-79-9 (EC No 268-093-2), 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., triesters with trimethylolpropane, CAS No 68002-79-9 (EC No 268-093-2), 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.

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

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, ECHA received comments from the Registrant.

On 7 January 2013, the Registrant updated his registration dossier (submission number [REDACTED]). On 4 March 2013, the Registrant updated his registration dossier another time (submission number [REDACTED]). On 22 March 2013, the Registrant updated his registration dossier yet again (submission number [REDACTED]). On 25 March 2013, the Registrant updated his registration dossier yet another time (submission number [REDACTED]).

ECHA considered the Registrant's comments and 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.

## 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;
- c. Description of the analytical methods or the appropriate bibliographical references for the identification of the substance (Annex VI, 2.3.7.), as described 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 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 1000 tonnes or more per year in accordance with Article 6 of the REACH Regulation, does not comply with the requirements of Article 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" thereafter. 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)), including also the assigned CAS identifier (as indicated in point (ii) thereafter).

#### (i) The manufacturing process

The fatty acids starting material used to manufacture the registered substance has not been identified to a sufficient level of detail in the dossier initially submitted. ECHA pointed out in its draft decision that UVCB substances such as this starting material cannot be sufficiently identified by a chemical name only. As the composition of such starting material is to a significant extent known and is one of the factors determining the composition of the registered substance, compositional information of that starting material (in terms of identity and upper and lower concentration levels of the different carboxylic acids) is a necessary element for its identification and therefore for the identification of the registered substance itself. ECHA thus requested, in its draft decision, the Registrant to provide detailed overall compositional information of the fatty acids starting material.

ECHA notes that the Registrant specified, in a registration update following the notification of the draft decision (thereinafter the "update dossier"), compositional information of the fatty acids both in the description field in IUCLID section 1.1 and in IUCLID section 3.1 of the dossier. However, discrepancies exist in the information provided. In particular, IUCLID section 1.1 indicates that the contribution of the linear saturated C18 carboxylic acid in the overall composition of the fatty acid starting material can reach up to ■■■ while the information in IUCLID section 3.1 indicates that the concentration in this constituent cannot exceed ■■■. Similar discrepancies also exist for the linear saturated C16 and the linear mono-unsaturated C16 carboxylic acids.

ECHA therefore concludes that the Registrant did not provide, in the update dossier, appropriate information on the overall composition of the fatty acids starting material, which was requested in the draft decision.

The Registrant is accordingly required to revise the compositional information reported for the fatty acids starting material, as specified in the first bullet point of sub-section (iii) below.

(ii) The CAS information

The chemical name reported by the Registrant in the dossier initially submitted indicated that the registered substance corresponds to esters of fatty acids comprising, in line with the Guidance, linear saturated carboxylic acids of even-numbered carbons. However, the CAS name of the CAS entry with CAS number 68002-79-9 assigned in the initial dossier did not specify that the constituents of the fatty acid starting material used in the manufacturing process were limited to carboxylic acids with even carbon numbers. 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 68002-79-9. 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 68002-79-9. 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 268-093-2 currently assigned to the substance (which is itself linked to the CAS number 68002-79-9) does not specifically correspond to the registered substance. The Registrant nevertheless maintained the CAS entry with CAS number 68002-79-9 under the "CAS information" header. In addition, the assigned CAS name makes reference to a carbon number range starting from C14 which is no longer quoted in the chemical name specified for the registered substance in the update dossier. 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 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

- Further detail on the manufacturing process must be provided

Based on the observation set out in sub-section (i) above, the Registrant is requested to submit consistent overall compositional information of the fatty acids starting material in terms of identity and upper and lower concentration levels of the individual saturated carboxylic acids and of each group of linear unsaturated carboxylic acids presenting the same carbon number.

The Registrant shall ensure that the chemical name assigned to the registered substance is consistent with the information on the manufacturing process.

Regarding in particular 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  $\geq 10\%$  (w/w) in the starting material); and
- the main groups of unsaturated fatty acids presenting the same carbon number (the "main groups" designating the groups with an upper concentration level  $\geq 10\%$  (w/w) in the starting material)

is considered 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  $\geq 80\%$  (w/w), this starting material shall be designated, in the chemical name of the registered substance, by the chemical name of that fatty acid. ECHA would like to stress that the Registrant shall ensure that this principle is complied with.

- 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 process. In these cases, 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. 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 manufacturing process description and any available CAS entry for the substance should be specified in the "Description" field and under the "CAS information" header in IUCLID section 1.1, respectively.

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. According to this information, the 2<sup>nd</sup>, 3<sup>rd</sup>, 4<sup>th</sup>, 5<sup>th</sup>, 6<sup>th</sup> and 7<sup>th</sup> listed constituents are derivatives of C17 unsaturated fatty acids and C15 saturated fatty acid. However, based on the manufacturing process description provided, such constituents with odd-numbered fatty acid blocks shall, in principle, not be present in the substance. In addition, these constituents are not observed in the analytical report attached in IUCLID section 1.4 of the dossier.

Furthermore, discrepancies exist on the stereochemistry of the unsaturation in at least the linear unsaturated C18 fatty acid moiety of the ester constituents. For the 1<sup>st</sup> listed constituent, the structural information indicates that the stereochemistry of that moiety is the Z isomer. However, for the other listed constituents including that block, the specified stereochemistry refers to the E isomer.

ECHA therefore concludes that the reported composition 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  $\geq 10\%$  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 unknown 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 these other constituents in 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 of the different saturated and unsaturated fatty acid blocks of the same carbon number (including C14 saturated linear, C16 saturated linear, C18 saturated linear, C16 unsaturated linear, C18 unsaturated linear as well as any other acid block also present) 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.

(c) Description of the analytical methods (Annex VI, section 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 noted that the Registrant provided, in the original dossier, the report from a gas chromatographic (GC) analysis of a sample of the registered substance that had been derivatised by a silylation reagent. This report included a peak table where peaks had been assigned to groups of constituents. The percentage of the constituents had also been reported, without any unit, in the table. However, the analytical report did not provide details of the method used for the identification of these groups of constituents. Furthermore, there was no information on the protocol followed to translate the results from the chromatographic analysis into concentration values of the groups of constituents present in the derivatised sample and of the constituents present in the composition of the registered substance itself.

In addition, ECHA observed that the original dossier did not include any description of the analytical methods used for quantifying the contribution of the different saturated and unsaturated fatty acid blocks presenting the same carbon chain length (including C14 saturated linear, C16 saturated linear, C18 saturated linear, C16 unsaturated linear, C18 unsaturated linear as well as any other acid block also present) within the ester constituents. ECHA thus requested the Registrant to provide the missing description of the analytical methods for the identification and quantification of the constituents and groups of constituents required to be reported in the composition.

ECHA notes that the Registrant replaced, in the update dossier, the original GC report by a report consisting in the gas chromatography- mass spectroscopy analysis of the registered substance. The Registrant used this new report to establish the composition of the registered substance. Whilst the report enabled the Registrant to characterise ester derivatives of the saturated C12, C16 and C20 and mono-unsaturated C18 fatty acids, it is unclear why esters of other fatty acids present in the composition of the starting material, such as the mono-unsaturated C16 and di-unsaturated C18 are not reported. ECHA underlines that, according to the compositional information of the fatty acid starting material, these latter two fatty acids are expected to contribute to a higher extent than e.g. the saturated C12 and C20 to the structure of the ester constituent of the registered substance.

ECHA therefore concludes that the Registrant did not provide, in the update dossier, an appropriate description of the analytical methods for the identification of the registered substance.



The Registrant is accordingly requested to clarify these discrepancies. The Registrant shall ensure that the description of the analytical methods used for the identification of the registered substances addresses the identification and quantification of all 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.

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 the 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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