ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114309015-64-01/F Helsinki, 24 September 2015

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

**For Fatty acids, C6-18, triesters with trimethylolpropane, CAS No 91050-88-3 (EC No 293-035-8), 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 Fatty acids, C6-18, triesters with trimethylolpropane, CAS No 91050-88-3 (EC No 293-035-8), 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 [redacted], for the tonnage band of 1000 tonnes or more 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 2 February 2015.

On 30 March 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 05 May 2015 ECHA received comments from the Registrant on the draft decision.

The ECHA Secretariat considered the Registrant's comments.
On basis of this information, Section II was amended. The Statement of Reasons (Section III) was changed accordingly.

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, 2.1.), as specified under section III.A.1 below;
2. Composition of the substance (Annex VI, 2.3.), as specified under section III.A.2 below;
3. High-pressure liquid chromatogram, gas chromatogram (Annex VI, 2.3.6.), as specified under section III.A.3 below;
4. Description of the analytical methods or bibliographical references (Annex VI, 2.3.7.), as specified under section III.A.4 below.

**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 **4 January 2016** 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). The naming of UVCB substances such as the registered substance shall consist of two parts: (i) the chemical name and (ii) a 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: 1.3, February 2014) - referred to as "the ECHA Guidance" hereinafter. According to the ECHA Guidance, the description of the manufacturing process shall include information on the chemical identity of the starting materials and information on the most relevant steps of the process.

However, ECHA observes that the Registrant did not provide sufficient information on the manufacturing process description to allow for an accurate and complete identification of the registered substance, as explained below.

More specifically, ECHA observes that the manufacturing process descriptions included in IUCLID Sections 1.1 and 3.1 do not sufficiently describe the identity of the starting materials and the ratio of the reactants used in the manufacturing process. In both IUCLID sections, the starting material carboxylic acids are described as "[redacted]" without specifying the exact identities and compositions of the "[redacted]" effectively used in the process. The chemical name assigned by the Registrant to the registered substance "Fatty acids, C6-18, triesters with trimethylolpropane" indicates that the substance corresponds to the triesters of linear C6-18 fatty acids with trimethylolpropane. ECHA understands that such fatty acids refer to a starting material comprising, in line with the ECHA Guidance, all linear carboxylic acids with chain lengths between C6–C18. Furthermore, the composition reported in section 1.2 suggests that [redacted] and "[redacted]" are used as the fatty acid starting materials. However, no further information has been provided on the identities and compositions of the fatty acid starting material(s).

ECHA points out that UVCB substances such as, in this case, the starting material(s) can not be sufficiently identified only by a generic description "[redacted]". As the composition of such starting material(s) 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 each individual linear carboxylic acid and of each group of unsaturated carboxylic acids, if present, presenting the same carbon number) is a necessary element for its identification and therefore for the identification of the registered substance itself.

Other elements of the manufacturing process description which are essential for the identification of the registered UVCB substance are also missing from the dossier. In particular, the ratio of reactants used for the manufacturing of the substance has not been reported. Both the ratios of the fatty acids used in the process and the ratio of the fatty acids to trimethylolpropane are missing. ECHA points out that the identity and ratio of reactants are essential elements of the manufacturing process as they determine the composition of the registered substance. In the absence of this information, it is not possible to verify the carbon number range or the level of saturation/unsaturation in the substance based on the manufacturing process.

Furthermore, ECHA notes that the information provided by the Registrant on the composition of the registered substance, as is explained below in section III.A.2, indicates that several substances may be covered by the registration. A detailed description of the manufacturing process, including the chemical identity of the source and information on the most relevant steps of the manufacturing process, is therefore required.

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

In line with the above observations and pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the missing information on the manufacturing process description. This information shall include:

- Compositional information of the starting material fatty acids in terms of identity and upper and lower concentration levels of each individual linear carboxylic acid and of

each group of unsaturated carboxylic acids (if present) presenting the same carbon number, and
- Ratios of all reactants.

If the substance covered by the registration is manufactured according to different manufacturing processes, including the use of different sources, then the detailed description of the manufacturing process(es) required hereinabove shall be reported separately for each manufacturing process. A manufacturing process may be considered different when the relevant 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.

The Registrant shall ensure that appropriate identifiers are assigned to the registered substance. It should be noted that the current chemical name (and EC and CAS identifiers) assigned to the registered substance do not take into account that only even-numbered alkyl chains are present in the substance as is reported in section 1.2 of the IUCLID dossier. Furthermore, the carbon number range and information on saturation/unsaturation (of the starting material if named according to this) needs to be appropriately reflected in the name.

The draft decision included instructions on how to take into account the compositional information of the fatty acid starting material(s) in the chemical name of the registered substance to be specified in the IUPAC name field of IUCLID. These instructions were relying both on the ECHA Guidance and on the *"OECD Guidance on Characterising Oleochemical Substances for Assessment Purposes"* (ENV/JM/MONO(2014)6, March 2014). The OECD document contains more specific instructions for deriving alkyl group descriptors for oleochemicals than does the ECHA Guidance.

In his comments to the draft decision, the Registrant pointed out that a different name is obtained by following the approach relying both on the ECHA Guidance and on the OECD document, than by relying only on the concepts included in the ECHA Guidance. As a result of the Registrant's comments, the following text on the derivation of the name has been modified, and it is to be considered as a recommendation.

Regarding the compositional information of the fatty acid starting material(s) and its designation in the chemical name of the registered substance specified in the IUPAC name field of IUCLID, ECHA points out that constructing the chemical name of the starting material(s) 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 starting material. 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.

This approach for deriving the chemical name of the registered substance reflects the specifications of the OECD Guidance. It is also not contradicting the permissible variations specified in the ECHA Guidance for substances for which the composition is to a significant part known (as it can be considered the case for the fatty acid starting material(s)). It also gives more flexibility regarding the carbon numbers present at a maximum concentration of <10% in the starting material. The Registrant is invited to consult the OECD Guidance for full details regarding this aspect. The Registrant should describe in the updated dossier the approach used in deriving the chemical name of the substance to be included in the IUPAC name field in section 1.1 of the IUCLID dossier.

In the comments to the draft decision the Registrant agreed with the information requirements in the draft decision. In addition, he indicated his intention to address the information requirements in an update of the registration after publication of the decision.

In the comments, the Registrant explained that he will update the manufacturing process description by including in sections 1.1 and 3.1 of the IUCLID dossier information on the starting material fatty acid carbon number distribution, and on the ratios of reactants, and provided this information already in the comments. Furthermore, the Registrant indicated that he would prefer to use the chemical name "[redacted]" derived in line with the OECD guidance from the fatty acid distribution of the starting material(s) and on the chromatographic analysis of the substance.

The information in the comments appears to be in line with the expectations in the draft decision. However, the information to be provided by the Registrant upon receipt of the final decision will be assessed on the basis of the updated dossier.

Regarding how to report the description of the manufacturing process of the UVCB substance, the information shall be included in the Description field in IUCLID section 1.1.

If the current numerical identifiers (EC number and CAS number) and the chemical name do not correctly identify the registered substance, they will need to be revised. The chemical name of the substance shall be included in the IUPAC name field in section 1.1 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." The CAS entry 91050-88-3 would need to be removed from the "CAS information" field if it is not appropriate for the substance and included in the "Related CAS information" field. The appropriate CAS entry that describes the substance identity, if available, shall be included in the "CAS information" field in section 1.1 of the IUCLID dossier. The Registrant shall note that the CAS entry used in the registration dossier (CAS number 91050-88-3) can cover substances that contain even numbered carboxylic acid groups and both even and odd carboxylic acid groups. The registration dossier can cover only one substance and it shall be clearly indicated to which substance it refers. This information must be consistent throughout the registration dossier.

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

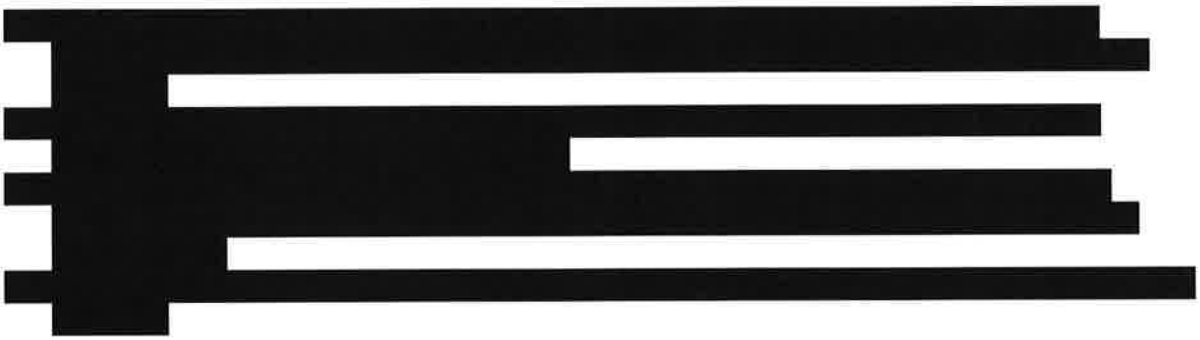
made.

2. Composition of the substance (Annex VI, Section 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, the Registrant reported in the composition included in section 1.2 of the IUCLID dossier the following four (groups of) constituents and concentration ranges:



The broad concentration range of [redacted] %(w/w) reported for the "Fatty acids, coco, triesters with trimethylolpropane" would indicate that the reported composition could cover at least two different substances:

- a substance predominantly derived from fatty acids other than those mainly found in "[redacted]", i.e. mainly from octanoic and decanoic acids when the concentration of this group of constituents is close to the minimum value of [redacted]%; and
- a substance predominantly derived from fatty acids including those mainly found in "[redacted]", when the concentration of this group of constituents is close to the maximum value of [redacted]%.

Furthermore, it is concluded by ECHA that the group of constituents "[redacted]" does not exist as such in the substance. Based on the process description, the "[redacted]" used as starting materials react with trimethylolpropane in the same process step. In the esterification, trimethylolpropane molecules will react with different fatty acids regardless of their origin, and it is not possible to pinpoint in the final substance whether the fatty acid blocks in the triesters would have originated specifically from "[redacted]", or from other fatty acids used as starting materials. Therefore, the group of constituents "[redacted]" cannot be reported separately as such in the composition.

It is also noted by ECHA that the typical concentrations reported for the (groups of) constituents included in section 1.2 amount in total to only [redacted] %(w/w), which indicates that at least [redacted]% of the composition has not been accounted for.

ECHA therefore concludes that the compositional information has not been provided to the required level of detail.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant shall revise the composition in section 1.2.

According to chapter 4.3 of the ECHA Guidance, the Registrant should note that, for UVCB substances presenting a large number of constituents 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
- Other 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 these other constituents in the substance which is the subject of this registration, the reporting of the unreacted fatty acids under one group and the reporting of the ester functionalised constituents according to groups presenting the same level of esterification (i.e. mono-esters, di-esters and tri-esters as applicable) is necessary for this aforementioned purpose. For each group of constituents, information on the relative abundance of the different linear saturated acid blocks and of the linear unsaturated acid blocks presenting 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.

The concentration range values must be representative for the registered substance as manufactured and it shall be clarified how the minimum and maximum values for each (group of) constituents were obtained (i.e. information on the batch selection, sampling procedure, the measured values, calculations used etc.). Without this information ECHA is not able to conclude on the representativeness of these values.

ECHA notes that, in the event the Registrant covers different grades of the registered substance in the present registration dossier, he shall report separately the compositional information of each grade. This means that if the substance covered by the present registration has two (or more) different compositions, then these must be presented separately. ECHA highlights that failure to report separately the compositional information of each grade of a substance may result in one or more grades not being covered by this registration.
In the comments to the draft decision the Registrant agreed with the information requirements in the draft decision. In addition, he indicated his intention to address the information requirement in an update of the registration after publication of the decision.

In the comments, the Registrant has explained how he will update the composition in section 1.2 of the IUCLID dossier, and has as well provided new information that has not been available earlier.

The information in the comments appears to be in line with the expectations in the decision. However, the information to be provided by the Registrant upon receipt of the final decision will be assessed on the basis of the updated dossier.

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, shall be reported in the appropriate fields in IUCLID. For the other constituents to be reported under a generic description, a generic chemical name describing the group of constituents, generic molecular and structural information (if applicable), as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID. The generic group of constituents "[redacted]" shall be divided into more specific (groups of) constituents. The relative abundance of the different fatty acid blocks within each group of ester constituents should be provided in the Remarks field of the repeatable block for that group of constituents.

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.

The Registrant shall ensure that there is sufficient analytical information included in Section 1.4 of the IUCLID dossier to identify and quantify the substance and to verify the information in Section 1.2.

3. High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.)

"High-pressure liquid chromatogram, gas chromatogram" is an information requirement as laid down in Annex VI, Section 2.3.6. 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 has not included sufficient chromatographic data required for the identification and quantification of the registered substance.

More specifically, ECHA notes that the copy of a gas chromatogram required to be provided according to Annex VI section 2.3.6. has been attached to the dossier (attachment "[redacted]"). This attachment includes also a results table indicating the contents of different types of ester groups divided according to the type of ester (mainly tri-esters) and the total carbon number of the carboxylic acid blocks in the tri-ester.

However, the Registrant did not provide a comprehensive report from the chromatographic analysis. In particular, the results table does not include the retention times of the peaks, the peak areas or a proper assignment of the peaks to constituents present in the substance. The table reported together with the copy of the chromatogram, where concentration values of constituents listed according to the ester type and total carbon number, can not be correlated to that chromatogram as there is no information as to how the listed constituents relate to the detected peaks. ECHA points out that a report of the chromatographic analysis in the form of a table with the peak list and peak areas is essential as it constitutes a numerical representation of the chromatogram. Without this information it is not possible to verify the composition of the substance.
Accordingly, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is

requested to provide the full report from the gas chromatographic analysis of the registered substance, including the retention times of the peaks, the peak areas, the peak assignments and the corresponding concentrations of (groups of) constituents in the substance.

In the comments to the draft decision the Registrant agreed with the information requirements in the draft decision. In addition, he indicated his intention to address the information requirement in an update of the registration after publication of the decision.

In the comments, the Registrant has explained how he will update the chromatographic information in section 1.4 of the IUCLID dossier, and has as well provided new information that has not been available earlier.

The information in the comments appears to be in line with the expectations in the decision. However, the information to be provided by the Registrant upon receipt of the final decision will be assessed on the basis of the updated dossier.

As for the reporting in the registration dossier, the information should be included in IUCLID section 1.4.

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

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 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.

More specifically, ECHA observes that the Registrant provided information on an analytical method used for the quantification of different esters present in the composition based on gas chromatography. The Registrant provided both a print-out of the chromatogram and a table listing different (groups of) esters identified according to the total carbon number of the carboxylic acid blocks together with their respective concentrations (in weight %). However, the Registrant did not include any description of the experimental protocol followed for the identification of the listed (groups of) constituents and for the calculation of their concentrations.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested 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.

In the comments to the draft decision the Registrant agreed with the information requirements in the draft decision. In addition, he indicated his intention to address the information requirement in an update of the registration after publication of the decision.

In the comments, the Registrant has explained how he will update the description of the chromatographic method in section 1.4 of the IUCLID dossier, and has as well provided new information that has not been available earlier.

The information in the comments appears to be in line with the expectations in the decision. However, the information to be provided by the Registrant upon receipt of the final decision will be assessed on the basis of the updated dossier.

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

Authorised[1] by Ofelia Bercaru, 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.