ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114306076-59-01/F Helsinki, 31 August 2015

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

For 1,2,3,6-Tetrahydrophthalic anhydride, oligomeric reaction products with 2,2-dimethylpropane-1,3-diol, EC No 500-091-1 (CAS No 36621-20-2), 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 for 1,2,3,6-Tetrahydrophthalic anhydride, oligomeric reaction products with 2,2-dimethylpropane-1,3-diol, EC No 500-091-1 (CAS No 36621-20-2), submitted by [redacted] (Registrant).

The scope of this compliance check decision is limited to the standard information requirements of Annex VI, Section 2 of the REACH Regulation.

This decision is based on the registration as submitted with submission number [redacted], for the tonnage band 100 to 1000 tonnes per year. This decision does not take into account any updates after the date when the draft decision was notified to the Registrant under Article 50(1) of the REACH Regulation.

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

The compliance check was initiated on 9 March 2015.

On 21 April 2015 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision.

By 28 May 2015 the Registrant did not provide any comments on the draft decision to ECHA.

On 11 June 2015 ECHA notified the Competent Authorities of the Member States of its draft decision and invited them pursuant to Article 51(1) of the REACH Regulation to submit proposals for amendment of the draft decision within 30 days of the receipt of the notification.

As no proposal for amendment was submitted, ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

II. Information required

A. Information in the technical dossier related to the identity of the substance

Pursuant to Articles 41(1), 41(3), 10(a)(ii) and Annex VI, Section 2 of the REACH Regulation the Registrant shall submit the following information for the registered substance subject to the present decision:

1. Name or other identifier of the substance (Annex VI, Section 2.1.)
2. Composition of the substance (Annex VI, Section 2.3.)
3. High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.)
4. Description of the analytical methods (Annex VI, Section 2.3.7.)

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.

B. Deadline for submitting the required information

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

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.)

ECHA notes that the Registrant identified the registered substance as of Unknown or Variable composition, Complex reaction products of 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: 1.3, February 2014) – referred to as "the Guidance" thereinafter. According to the 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. Any other identifier, including any CAS number (if available) and any EC number (if available and appropriate) for the substance shall also be reported.

(i). The CAS number

The CAS entry assigned by the Registrant to the registered substance is linked to the EC number 500-091-1 also assigned by the Registrant to the substance. However, as specified on page 8 of the No-Longer Polymer (NLP) list (version 3, available on EU Bookshop website managed by the Publications Office of the European Union in Luxembourg at https://bookshop.europa.eu): "*NLP-Nos and name descriptions take precedence. The CAS-RN given are to be treated as indicative and for a use as a searching tool*". ECHA therefore considers that the CAS information included in the registration dossier is generic and does not fully correspond to the registered substance.

The Registrant is accordingly requested to delete the CAS number currently specified under the "CAS information" header of the reference substance in IUCLID section 1.1 and report a CAS number specifically corresponding to the registered substance (if available). If the Registrant deems it appropriate, he may specify the current CAS entry as "related CAS information" for the registered substance.

(ii). The manufacturing process

The chemical name assigned by the Registrant to the registered substance and the description of the manufacturing process provided indicate that the registered substance corresponds to a complex set of constituents resulting from the oligomerisation of 1,2,3,6-tetrahydrophthalic anhydride and 1,2-dimethylpropane-1,3-diol.

Section 3.1 of the IUCLID dossier furthermore specifies that "[redacted]". However, no information has been provided on the manufacturing process.

ECHA however considers that the description of the manufacturing steps reported in the dossier is not sufficiently detailed for the following reasons:

- According to the second listed composition in section 1.2 of the IUCLID dossier, the registration covers a substance which can include a significant concentration level (up to [redacted]%) of the constituent or group of constituents "tetrahydromethylphpthalic anhydride" with unspecific position of the double bond and the methyl substituent on the cyclohexylphthalic anhydride backbone. The origin of this group of constituents can however not be explained by the submitted description of the manufacturing process. In particular, the origin of the methyl substituent and the unspecific position of the double bound cannot be predicted from the reactions expected to take place between 1,2,3,6-tetrahydrophthalic anhydride and 1,2-dimethylpropane-1,3-diol. The presence of such constituents would indicate the use of additional/alternative starting materials and/or the application of additional processing steps beyond what was described by the Registrant in the registration for the manufacturing of the substance.
- The relative ratio of each reactant has not been specified;
- The process parameters used to control the composition have not been clearly reported. ECHA notes that the Registrant made reference to the use of elevated temperature and the possible use of catalyst. It is however unclear how these specifications of the process are eventually adjusted to control the composition;
- The Registrant did not describe the steps applied to isolate the substance, including any eventual purification steps undertaken.

ECHA points out that UVCB substances such as the registered substance cannot be sufficiently identified by the chemical names of the starting materials only. As the abovementioned missing elements of the manufacturing process are expected to determine the composition of the registered substance, and taking also into account the limited information on the composition of the registered substance in the current dossier (see section III.A.2 herein below), ECHA considers that these elements are necessary for the identification of the registered 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 substance.

The Registrant is accordingly required to provide details of the manufacturing processing steps that are applied to the starting materials. The information submitted by the Registrant must at least include the following:

- The identity of all the starting materials used for the manufacturing of the registered substance.
- The molar ratio of between the different starting materials used.
- A description of the manufacturing steps in the order they occur, including any preliminary step, the steps involving chemical transformation as well as the isolation and purification steps carried out for the synthesis.
- For each step, all relevant process parameters that affect the composition and therefore the identity of the substance must be provided.

Regarding more specifically the steps involving a chemical transformation, the Registrant shall provide a description of the relevant oligomerisation steps, including the parameters used to initiate, propagate and terminate the oligomerisation reactions. The Registrant shall also report the reaction mechanisms taking place for the manufacturing. The report of these mechanisms shall be sufficient to reason the presence of the constituents present in the composition required to be reported in the dossier.

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 source, manufacturing process 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.

The Registrant shall also note that substances manufactured according to different manufacturing processes may indicate multiple substances and consequently the requirement for multiple registrations. ECHA has set up a process enabling registrants to adapt their registration in such cases. 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 for the registered substance shall be reported in the "Description" field of the reference substance in IUCLID section 1.1. Any CAS number specifically corresponding to the registered substance shall be reported under the "CAS information" header of the reference substance in IUCLID section 1.1.

The Registrant shall ensure that the chemical name and other identifiers reported in section 1.1 of the IUCLID dossier are consistent with the substance as described by the manufacturing process and are representative of its composition. The Registrant shall note that the registration is currently linked to EC number 500-091-1 referring to the oligomerisation reaction products between 1,2,3,6-tetrahydrophthalic anhydride and 1,2-dimethylpropane-1,3-diol. Should the substance intended to be covered by this registration refer to a different substance, the Registrant can however not remove or modify at this stage identifiers such as the EC number for technical reasons, the registration being linked to that number in REACH-IT. To ensure unambiguous identification of the registered substance, the Registrant shall however indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC number 500-091-1 currently assigned does not specifically correspond to the registered substance. This identifier cannot be modified or deleted at this stage in the present registration update for technical reasons". The Registrant shall also specify, in the same "Remarks" field, any available and appropriate EC number for the substance. The Registrant shall note that ECHA has established a process, subject to certain conditions, enabling registrants to adapt an existing registration, while maintaining the regulatory rights already conferred to the substance concerned.

The Registrant shall note that, for substances such as the registered substance, the use of different starting materials (e.g. the use of different anhydrides) would normally be expected to lead to the manufacturing of different substances. In addition, in line with the NLP list, "*Mixture of oligomers or isomer mixtures are generally listed in the no-longer polymer list with the name of the main component only when present in the mixture with*

80% or more", the "main component" designating in this case constituents or a group of constituents presenting the same level of oligomerisation (e.g. monomers, dimers, trimers). Accordingly, oligomers with different main components would normally be regarded as different substances. Furthermore, if the manufactured substance does not predominantly consist of oligomerisation reaction products (i.e. these oligomerisation reaction products do not typically represent [redacted]% or more of the composition), it would normally be regarded as a different substance than the substance with EC number 500-091-1.

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.

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

Annex VI, Section 2.3. of the REACH Regulation requires that each registration dossier contains sufficient information for establishing the composition of the registered substance and therefore its identity.

In that respect, according to chapter 4.3 of the Guidance, the Registrant should note 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 by a generic description of their chemical nature.

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

In the present dossier, the Registrant reported two compositions: one composition typically consisting of [redacted]% of the substance itself, i.e. of the "*1,2,3,6-Tetrahydrophthalic anhydride, oligomeric reaction products with 2,2-dimethylpropane-1,3-diol*" and, the other with the same generic entry describing the oligomerisation reaction products but with a typical concentration of [redacted] % and another constituent or group of constituents (i.e. tetrahydromethylphthalic anhydride) of unclear origin with also a typical concentration of [redacted] %.

ECHA notes that the compositions provided by the Registrant are not sufficiently specific. More specifically, as mentioned in the Guidance above, the Registrant should have identified the unknown constituents by a generic description of their chemical nature which would include details on the distribution of molecular weight or the degree of oligomerisation by grouping different class of oligomers. Thus, the Registrant has not provided sufficient information for establishing the composition of the registered substance and therefore its identity.

ECHA also notes that the reported compositional information is inappropriate for the following reasons:

- The identity of the group of constituents "tetrahydromethylphthalic anhydride" is unclear. The assigned CAS number 11070-44-3 as well as the EC number 234-290-7reported in the Remarks field of the repeatable block for that

group indicated that it consists of tetrahydromethylphthalic anhydride isomers with unspecific position of the double bond and the methyl substituent. The molecular and structural information however refers to the structure "(3aR)-3a-methyl-3a,4,5,6-tetrahydro-2-benzofuran-1,3-dione" with specific position of the double bond and methyl group

- The typical concentrations for the constituents in second listed composition add up to [redacted]% and therefore overall exceed [redacted]%.

The Registrant is accordingly required to specify the identity and typical, upper and lower concentration level of the constituents and groups of constituents required to be reported. Concerning the reporting of the unknown constituents, the grouping of these constituents according to the level of oligomerisation and the identity of the terminal groups is necessary as a baseline.

The Registrant shall ensure that the identifiers reported for each constituent and group of constituent are consistent with each other and that the reported concentration levels do not add up to more ant [redacted]%. The Registrant shall also ensure to remove from the dossier any composition eventually referring to another substance than the substance which is the subject to this registration.

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.

Regarding how to report the composition in IUCLID, the following applies:

The Registrant shall indicate the composition of the registered substance in IUCLID Section 1.2.

For each constituent and group of constituents, the IUPAC name, CAS name and CAS number (if available), molecular and structural formula, as well as minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID.

For the unknown constituents to be reported under a generic description, a generic chemical name describing the group of constituents, generic molecular and structural information (if applicable), as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID.

Further technical details on how to report the composition of UVCB substances in IUCLID are available in paragraphs 2.1 and 2.2.2 of the Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH (Version: 2.0, July 2012) on the ECHA website. Information on how to report several compositions in IUCLID is specified in paragraph 2.3, Q&A 8 of that manual.

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

High-pressure liquid chromatogram (HPLC) or gas chromatogram (GC) is a formal information requirement of Annex VI, Section 2.3.6.

ECHA notes that the Registrant did not include any chromatogram for the registered

substance in the registration dossier.

ECHA regards this required information scientifically relevant for the registered substance as it provides a meaningful fingerprint for the identification of organic substances such as the registered substance.

The Registrant is therefore requested to submit the chromatographic data for the registered substance.

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 any 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.

The registrant attached IR, UV, NMR and MS spectral data in the registration dossiers. Whilst the results of these analysis may be used to identify the chemical functionalities/structures present in the composition of the analyses sample, they do not provide any information on the exact identity and actual concentration level of the constituents and groups of constituents required to be reported in the composition.

The Registrant is accordingly 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.

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

The Registrant shall ensure that the composition to 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 Claudio Carlon, Head of Unit, Evaluation

[2] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.