ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114310551-65-01/F Helsinki, 10 December 2015

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

For 4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane, reaction products with butan-1-ol and 3-arninomethyl-3,5,5-trimethylcyclohexylamine, EC No 500-652-0 (CAS No 161308-12-9), registration number: [redacted]

Addressee: [redacted]

The European Chemicals Agency (ECHA) has taken the following decision in accordance with the procedure set out in Articles 50 and 51 of Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH Regulation).

I. Procedure

Pursuant to Article 41(1) of the REACH Regulation ECHA has performed a compliance check of the registration for 4,4'-Isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane, reaction products with butan-1-ol and 3-arninomethyl-3,5,5-trimethylcyclohexylamine, CAS No 161308-12-9 (EC No 500-652-0), submitted by [redacted] (Registrant). The scope of this compliance check decision is limited to the requirements regarding the identification of the substance (Section 2 of Annex VI).

This decision is based on the registration as submitted with submission number [redacted], for the tonnage band of 100 to 1000 tonnes per year. This decision does not take into account any updates after 23 February 2015, i.e. 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 30 October 2014.

On 23 February 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 30 March 2015 ECHA received comments from the Registrant on the draft decision.

The ECHA Secretariat considered the Registrant's comments. The information is reflected in the Statement of Reasons (Section III) whereas no amendments to the Information Required (Section II) were made.

On 3 September 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

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

Pursuant to Articles 41(1)(a), 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.);
2. Composition of the substance (Annex VI, 2.3.);
3. Description of the analytical methods (Annex VI, 2.3.7.).

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated registration to ECHA by **17 March 2016.**

III. Statement of reasons

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

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.

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, 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 substance (as explained under points (i) and (ii) hereinafter).

(i) Information on the chemical name and numerical identifiers to be submitted by the Registrant

ECHA notes that the chemical name specified assigned by the Registrant in the registration dossier would indicate that the registered substance is the result from the reaction between [redacted]. The same observation can be made with the chemical names associated to the EC number 500-652-0 and CAS number 161308-12-9 also specified in the dossier. However, the following ambiguities in the registration dossier prevent ECHA from concluding on the appropriate and representative chemical name and numerical identifiers for the registered substance:

- The CAS name of the CAS entry 161308-12-9 used by the Registrant generically refers to a polymer whereas the EC name of the assigned EC entry 500-652-0 used by the Registrant refers more specifically to an oligomeric substance which does not meet the polymer definition specified in Article 3(5) of the REACH Regulation. Even though the EC entry 500-652-0, which is included in the No-Longer Polymer (NLP) list (available on esis.jrc.ec.europa.eu website), is actually linked to the CAS entry 161308-12-9, the Registrant shall note that the NLP list specifies that "*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*" (see page 8 of the document). ECHA therefore considers that the CAS information included in the registration dossier is generic and does not fully correspond to the registered substance.

- According to the manufacturing process description reported in sections 1.1 and 3.1 of the IUCLID dossier, one of the starting materials is designated as the well-defined substance [redacted]. However the chemical identifiers assigned to the registered substance describe the starting material as a UVCB substance [redacted] and therefore a different starting material than the well-defined substance [redacted]. The same contradiction can be found in the table from chapter 1 of the analytical report attached in IUCLID section 1.4.

- According to the manufacturing process description, [redacted] is charged together with [redacted] into the reactor containing [redacted]. However, the chemical identifiers assigned to the registered substance refer instead to a substance obtained by reacting [redacted] and [redacted] with "[redacted]. The reaction products from these two different processes are not expected to be chemically equivalent.

- The chemical name specified by the Registrant and the chemical names associated to the assigned EC and CAS numbers do not describe the chemical nature of the registered substance. Whilst they refer to the substance as oligomerisation (or polymerisation) reaction products, the substance would include, according to the composition reported in the dossier, a significant proportion (up to [redacted]% w/w) of unreacted [redacted].

For these reasons the chemical name and identifiers cannot be considered appropriate at this stage based on the information provided in the dossier.

Accordingly, the Registrant is required to clarify the identity of the registered substance by providing a chemical name which reflects the chemical nature of the registered substance and includes the specific IUPAC names (or the specific chemical names derived according to the Guidance) of the starting materials used, in line with the naming conventions specified in the Guidance for substances such as the registered UVCB substance.

The Registrant shall also delete the CAS number currently specified under the "CAS information" header of the reference substance in IUCLID section 1.1 and report instead available CAS number specifically corresponding to the registered substance.

As for the reporting of the information in IUCLID, the IUPAC name shall be reported in the "IUPAC name" field and under the "CAS information" header of the reference substance in IUCLID section 1.1. The CAS entry with CAS number 161308-12-9 may be reported under the "Related CAS information" header in IUCLID section 1.1.

If the EC entry assigned in the registration dossier does not fully correspond to the registered substance (e.g. if the EC entry does not reflect the identity of the starting materials used, the order of reactions applied and/or the description of the substance as consisting of oligomerisation reaction products), the Registrant shall not remove or modify at this stage this EC entry for technical reasons, the registration being linked to that EC entry in REACH-IT. To ensure unambiguous identification of the registered substance, the Registrant shall however specify in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 500-652-0 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 should note that ECHA has established processes, subject to certain conditions, enabling registrants to adapt the EC identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned. Should the Registrant consider that the EC identifier provided in his dossier should be adapted to cover a different substance or if it actually covers several other substances, he is thus encouraged to contact ECHA for a possible adaptation of the registration.

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

(ii) A detailed manufacturing process description to be submitted by the Registrant

Based on the information provided by the Registrant regarding the composition of the registered substance, ECHA concludes that the exact identity and concentration levels of the individual constituents reported in section 1.2 of the updated dossier are not sufficiently known for the UVCB substance to be identified by its composition alone. ECHA also underlines that the chemical name used by the Registrant to identify the registered substance, which is based on its starting materials, does not allow for an accurate and complete identification of the substance. A detailed

description of the manufacturing process, including the chemical identity of the starting materials and information on the most relevant steps of the manufacturing process, is therefore required.

However, the information provided by the Registrant on the manufacturing process is not sufficiently detailed and appropriate for the identification of the registered substance.

In particular, as already mentioned in section A.1.(i) hereinabove in this decision, the registration dossier includes contradicting information on the identity of the reactants used and the order of the manufacturing processing steps applied. In addition, the description does not include the following information which normally influences the composition of the registered substance and therefore is necessary for the identification of the registered UVCB substance:

- the exact ratio of reactants used. ECHA notes that the Registrant indicated that an excess of [redacted] is used in the process. However, the reactant(s) to which [redacted] is used in excess is unclear. The relative ratio of the other reactants used has also not been specified;
- the reaction type(s) involved in the manufacture the substance
- Specifications of relevant manufacturing process parameters (e.g. temperature, pressure, solvent used, if any) applied to each step as well detailed of information on any purification step(s) and the isolation step(s) applied.

The Registrant is accordingly required to provide the abovementioned missing information on the manufacturing process.

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.

The Registrant shall ensure that the chemical name, the identifiers and the manufacturing process description to be reported according to Annex VI, Section 2.1 are consistent with each other and with the composition required to be provided according to Annex VI, Section 2.3.

In the comments to the draft decision, the Registrant agreed to clarify the identity of the registered substance, in line with the naming conventions specified in the Guidance. The Registrant also agreed to provide information on the chemical name and numerical identifiers and to provide a detailed manufacturing process description. The information to be provided by the Registrant will only be assessed on the basis of an updated dossier.

2. Composition of the substance (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 cornerstone of all the REACH obligations.

ECHA notes that the registration does not contain sufficient and appropriate 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 notes the following:

- The identity of the groups of constituents referred to by the Registrant as [redacted] is unclear. The Registrant did not provide any structural representation of these groups of constituents in section 1.2 of the IUCLID dossier. Whilst structures have been included in the analytical report [redacted] under [redacted], it is not clear how far these structures are representative of the constituents actually covered by these two groups;

- The Registrant did not specify the cis/trans ratio of the residual [redacted]. The provided High Performance Liquid Chromatography - Evaporative Light Scattering Detector (HPLC-ELSD) chromatogram shows [redacted] peaks in the region around the peaks derived from [redacted]. Normally [redacted] peaks corresponding to the 2 pairs of enantiomers would be expected to be found under the applied analytical recording conditions;

- The reported composition in section 1.2 of the IUCLID dossier is not in line with the results of the HPLC-ELSD analysis for the [redacted]. The area % of the peaks in the chromatogram for this group of constituents is about [redacted]% as reported in the "Table of peaks and integration results" of the analytical report. However ≥ [redacted]% of such "oligomeric species" is stated in IUCLID Section 1.2.

- The Registrant did not specify separately the concentration levels of the [redacted] and [redacted] adducts.

According to chapter 4.3 of the Guidance, for UVCB substances such as the registered substance, the Registrant shall note the following:

- All constituents present in the substance with a concentration of ≥ 10 % shall be identified and reported individually;
- All known constituents and constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually; and
- Unknown constituents shall be identified as far as possible by a generic description of their chemical nature. The identification of these other constituents must be provided in order to allow ECHA to establish the composition of the substance as manufactured and to use the compositional information as one identifier for the registered substance. This information must also allow ECHA to verify that the composition is consistent with the chemical name reported for the registered substance. Regarding the reporting of unknown oligomeric constituents, a distinction according to the identity, sequence and number of units which these constituents consist of and to the type of termination is normally required for this purpose as a baseline.

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

The Registrant is accordingly required to revise the composition by providing the missing structural information. The Registrant shall also clarify the isomerism of the residual [redacted] and specify its cis/trans ratio. The Registrant shall also clarify the concentration level of the reported constituent [redacted] in section 1.2. The Registrant shall report separately the [redacted] and [redacted] adducts and specify their concentration levels.

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).

In the comments to the draft decision, the Registrant agreed to clarify the substance composition. The information to be provided by the Registrant will only be assessed on the basis of an updated dossier.

3. 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 different constituents present in the composition of the registered substance, which is requested according to Annex VI section 2.3.7.

More specifically ECHA notes that the description of the HPLC-ELSD analytical method used for the identification and quantification of the constituent(s) is not sufficiently detailed in the dossier. The Registrant provided ELSD calibration curve for [redacted] only but not for the higher molecular weight (MW) oligomers. Therefore the quantification of these species is not well reflected in the analytical report. It is unclear how the concentrations reported in section 1.2 of these oligomers were calculated from the provided "% Area" values.

The Registrant is accordingly required to provide a proper description of the analytical methods used for the identification and quantification of all individual constituents and groups of constituents required to be reported. 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 explained that it was not possible to quantify oligomers separately because of absence of standards.

ECHA acknowledges the possible limitation of evaporative light scattering as a quantitative detection technique without the use of standards, taking into account the dependence of the ELSD detector's response to the mobile phase composition. In this case, the mobile phase composition varies from the outset with the use of a gradient elution. ECHA would like to clarify that the Registrant is in principle not limited to the use of this specific method or this experimental protocol to establish the composition of the registered substance. The use of a different detector or different analytical techniques may also be considered to obtain an appropriate quantitative estimation of the eluted constituents even in absence of a specific standard. Regardless of the analytical method followed, any uncertainty in the quantification of the substance should in principle be taking into account in the concentration ranges of the constituents to be reported in the composition.

ECHA also takes note of the commitment from the Registrant in the comments to the draft decision to identify the constituents as far as possible by a generic description of their

chemical nature and to revise the composition by providing the missing structural information. The Registrant shall ensure to include in the registration the description of the analytical method(s) applied for establishing the composition of the registered substance to this level of detail. The information to be provided by the Registrant will only be assessed on the basis of an updated dossier.

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 E3

[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.