EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114322749-42-01/F Helsinki, 27 May 2016

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

For [redacted], EC No [redacted], 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 Reaction mass of 2-methylpentane and Hexanol, branched and linear and diisopropyl ether, EC No 906-390-7, 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 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 23 September 2015.

On 27 October 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 23 November 2015 ECHA received comments from the Registrant on the draft decision.

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

On 21 January 2016 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.
Subsequently, no proposals for amendment to the draft decision were submitted.

ECHA took the decision pursuant to Article 51(6) 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. Spectral data (Annex VI Section 2.3.5.)
4. High-pressure liquid chromatogram, gas chromatogram (Annex VI Section 2.3.6.)
5. Description of the analytical methods (Annex VI Section 2.3.7.)

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 **05 December 2016** 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.

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.)

Annex VI, section 2.1. of the REACH Regulation requires that the registration dossier contains adequate and sufficient information to enable each substance to be identified.

ECHA notes that the Registrant identified the registered substance as a well-defined multi-constituent substance. According to chapter 4.2 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.3, February 2014) – referred to as "the Guidance" thereinafter, well-defined substances are these with fully defined qualitative and quantitative composition.

Multi-constituent substances consist of several main constituents which are present at concentrations generally ≥ 10% and < 80% (w/w) and they are named as a reaction mass of two or more main constituents. Each constituent of a well-defined substance requires a complete chemical speciation, including structural information. This implies that constituents of well-defined substances must have a clearly defined chemical identity and a unique definitive molecular formula.

In the present dossier the Registrant identified the substance as a multi-constituent substance and indicated "[redacted]" as the chemical name of the registered substance. The Registrant states in the description field that the substance is a "*A complex and variable combination of hydrocarbons having carbon numbers predominantly in the C3, C6 & C9 chain length and oxygenated organic molecules, predominantly diisopropyl ether and hexanol (branched and linear).*"

The chemical name indicates that the registered substance has three main constituents "[redacted]. However, based on the analytical data provided [redacted] is present in the substance < [redacted]% (w/w) and therefore cannot be regarded as a main constituent. Furthermore [redacted] covers multiple constituents which based on the analytical data can be identified and quantified separately (e.g [redacted] and therefore should be also reported separately and not as a group of constituents. In addition it should be taken into account that "[redacted]" indicates that also [redacted] would be present in the registered substance, however based on the analytical information this is not the case.

Based on the analytical data provided there is potentially only one well-defined constituent ("[redacted]") present in the registered substance ≥ 10% and < 80% (w/w) and therefore only this constituent can be considered as a main constituent of the registered substance.

The information provided in IUCLID section 1.1 regarding the structural formula indicate that 17 different constituents are present in the substance and the results of the chromatographic analysis in IUCLID section 1.4 indicate the presence of 20 constituents or constituent groups. This information together with the description of the manufacturing process given in IUCLID section 3.1 ([redacted]) would indicate that the substance consists of multiple constituents, some of them not being well-defined, and therefore could be more appropriately identified as a Substances of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB).

ECHA therefore concludes that the substance has not been sufficiently identified and the chemical name currently used is inconsistent with the rest of the information given and as a result not representative for the registered substance.

Based on the information given, the substance could be more appropriately identified as a UVCB instead as a multi-constituent substance, because of the relatively large number of constituents and the potential variability of the composition.

Accordingly, the Registrant is requested to clarify the identity of the substance and ensure that the information is consistent throughout the dossier.

In case the Registrant decides to identify the registered substance as a multi-constituent substance, the main constituents present at concentrations generally ≥ 10% and < 80% (w/w) need to be taken into account when naming the substance and the generic format

used for naming multi-constituent substances is "Reaction mass of [IUPAC names of the main constituents]".

In case the Registrant decides to identify the registered substance as a UVCB substance, the following applies:

a) The naming of the UVCB substances consists 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.
b) The description of the manufacturing process shall cover the starting material used, ratio of the starting materials, steps and relevant process parameters. It needs to be taken into account that according to the Guidance any significant change of source or process would be likely to lead to a different substance that should be registered again. As a result the different glycols used in the process may result in different substances.

Regardless of the substance type chosen all identifiers given in section 1.1 needs to be consistent with each other.

As for the reporting of the information in IUCLID, the following applies: The Registrant shall decide first whether the substance is to be identified as a multi-constituent substance or a UVCB substance.

In case of a multi-constituent substance the substance is named as a "Reaction mass of [IUPAC names of the main constituents]" and this name is indicated in the IUPAC name field in IUCLID section 1.1. The main constituents shall be consistent with the constituents listed in IUCLID section 1.2 as "constituents".

In case of a UVCB substance the chemical name and the manufacturing process description shall be specified in the "IUPAC name" and "Description" field in IUCLID section 1.1, respectively.

Further technical details on how to include the name and report the composition of a multi-constituents substance or UVCB substances in IUCLID are available in paragraphs 2.1 and 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.

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

Annex VI, section 2.3. of the REACH Regulation requires that each registration dossier contain 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 for well-defined substances multi-constituent substances, the following applies:

- Each main constituent present at ≥ 10% (w/w) and < 80% (w/w) shall be identified and reported individually, with their typical concentration and concentration range;
- Each impurity present at ≥1% or relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually, independently from their concentration;
- Unknown constituents shall be identified by a generic description of their chemical nature.

In the present dossier, in IUCLID section 1.2 the Registrant reported the composition as "[redacted]" without any breakdown.

Based on the analytical data provided in IUCLID section 1.4, more specific information on the composition of the substance is available as the Registrant has provided a list of 20 constituents or constituent groups present in the registered substance together with their relative amounts and some of the constituenst are present at ≥[redacted]%.
However, these constituents have not been reported in IUCLID section 1.2.

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

Accordingly the Registrant is requested to clarify the composition of the substance.

In case the Registrant decides to identify the registered substance as a multi-constituent substance, it needs to be taken into account that each constituent of a well-defined substance requires a complete chemical speciation, including structural information. This implies that constituents of well-defined substances must have a clearly defined chemical identity and a unique definitive molecular formula.

When reporting the composition of a multi-constituent substance the following applies:

- Each main constituent present at ≥ 10% (w/w) and < 80% (w/w) shall be identified and reported individually, with their typical concentration and concentration range;
- Each impurity present at ≥1% or relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually, independently from their concentration;
- Unknown constituents shall be identified by a generic description of their chemical nature.

In case the Registrant decides to identify the registered substance as a UVCB substance, the following applies:

- All known constituents and all constituents present in the substance with a concentration of ≥ 10 % shall be identified and reported individually, with their typical concentration and concentration range
- All constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually, independently from their concentration; and
- Unknown constituents shall be identified by a generic description of their chemical nature.

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.

In case of a UVCB substance all constituents are to be listed under "constituents" as the terms "main constituents" and "impurities" are not regarded as relevant for UVCB substances.

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. While it might not be possible to identify each individual constituent of your substance due to their number and complexity, it should be possible to group and report for each group of constituents the carbon chain distribution and a distinction should be made also between linear and branched carbon chains.

The concentration range values of the constituents or groups of constituents must be representative for the inquired substance as manufactured/imported.

Further technical details on how to report the composition of a multi-constituent substance or 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.

3. Spectral data (Annex VI Section 2.3.5.)

Spectral data are an information requirement of Annex VI Section 2.3.5.

The Registrant has not provided spectral data (ultra-violet (UV), infra-red (IR), nuclear magnetic resonance or mass spectrum (NMR)) in the registration dossier.

ECHA regards this required information scientifically relevant for the registered substance for the following reasons:

- The substance absorbs in the UV range due to the presence of constituents containing chromophores. A UV spectrum representing the absorption of these constituents in the UV range can therefore be recorded;
- The IR spectrum displays characteristic vibration bands of covalent bonds in molecules present in the substance, including characteristic vibration bands from the chemical functionalities expected to be present in the composition;
- NMR spectroscopic analyses such as a 1H-NMR or a 13C-NMR are powerful tools for structure characterisation and elucidation due to characteristic chemical shifts and spin-spin coupling which also reflects the relative abundance of individual atoms.

The Registrant is therefore requested to provide a UV spectrum, an IR spectrum and an NMR spectrum, such as a 1H-NMR or a 13C-NMR. As an alternative to an NMR spectrum, mass spectra (MS) generated as part of mass spectroscopic analysis for the elucidation of the structure of the constituents in the substance can be provided.

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

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

Chromatographic data is an information requirement of Annex VI Section 2.3.6.

ECHA observes that the Registrant has provided a list of constituents with relative amounts, however the chromatogram and a peak table with the associated retention times and peak area have not been included.

ECHA regards chromatographic information scientifically relevant for the registered substance in order to confirm the composition of the substance.

Accordingly the Registrant is required to provide a high-pressure liquid chromatogram or gas chromatogram with a quantitative analysis enabling the identification of the substance composition.

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

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

Description of the analytical methods is an information requirement of Annex VI Section 2.3.7.

ECHA observes that the Registrant did not provide a description of the analytical method(s) used for the identification of the substance.

This information is essential to confirm the identity of the registered substance.

Consequently, the Registrant is requested to provide a description of the analytical method(s) used for the identification of the substance. The description shall be given in such detail that the method can be reproduced and shall therefore include a detailed experimental protocol. Typical results of the analysis should also be reported.

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

Deadline for submitting the required information

In the draft decision communicated to the Registrant the time indicated to provide the requested information was 3 months from the date of adoption of the decision. In his comments on the draft decision of 23 November 2015, the Registrant requested an extension of the timeline to 9 months (he requested 6 additional months over and above the standard 3 months). He sought to justify this request by stating that he proposes a revised identification, including sampling, analysis and re-submission. Taking into account the level of complexity of the substance identification, and taking into account that the substance is not part of a large category involving several registrants, ECHA considered it justified extending the deadline by 3 months.

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[2] by Claudio Carlon, Head of Unit, Evaluation E2

[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.