ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 10 August 2018

Addressee: [redacted]

Decision number: CCH-D-2114439546-42-01/F
Substance name: Acetic acid, oxo-, potassium salt, reaction products with ethylenediamine and para-hydroxybenzenesulfonic acid potassium salt, iron potassium salts
EC number: 462-490-6
CAS number: NS
Registration number: [redacted]
Submission number: [redacted]
Submission date: 25/07/2014
Registered tonnage band: 100-1000

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (the REACH Regulation), ECHA requests you to submit information on:

1. **Name or other identifier of the substance (Annex VI, Section 2.1.) of the registered substance;**

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

3. **Description of the analytical methods (Annex VI, Section 2.3.7.) on the registered substance;**

You have to submit the requested information in an updated registration dossier by **19 November 2018**.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2 and advice and further observations are provided in Appendix 3.

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

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, has to be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under: http://echa.europa.eu/regulations/appeals.

Authorised[1] by, Jos Mossink, Head of Unit, Substance Identification and Data Sharing, C2.

[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.

Appendix 1: Reasons

In accordance with Article 10(a)(ii) of the REACH Regulation, the technical dossier must contain information on the identity of the substance as specified in Annex VI, Section 2 to the REACH Regulation. In accordance with Annex VI, Section 2 the information provided has to be sufficient to enable the identification of the registered substance.

1. Name or other identifier of the substance (Annex VI, Section 2.1.)

The name and other identifiers (e.g structural formula) 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 registration dossier for the registered substance to meet this information requirement.

You 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: (a) the chemical name and (b) a more detailed description of the manufacturing process, as indicated in section 4.3 of the 'Guidance for identification and naming of substances under REACH and CLP' (May 2017, Version 2.1), referred hereafter as the Guidance.

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.

You provided a chemical name in the IUPAC name field ("Acetic acid, oxo-, potassium salt, reaction products with ethylenediamine and para-hydroxybenzenesulfonic acid potassium salt, iron potassium salts") and a description of the manufacturing process.

The provided manufacturing process description is in line with the chemical name but does not report information on the crucial parameters that might influence the composition of your substance, such as the identity of one of the starting materials used (described as an [redacted]), ratio of the reactants, pH values, reaction scheme etc. There is also no information on the neutralisation step of the ligand.

Therefore, the manufacturing process description is missing details on the starting materials and relevant steps of the process that are necessary to verify the identity and composition of the substance.

Additionally, the provided structural formula in section 1.1 of your dossier reports a deprotonated ethylenediamine moiety and consequently an unbalanced charge as the oxidation state of the iron is indicated to be +3 and the overall charge of the ligands is -6. However, this characteristic is not reflected in the name and manufacturing process of the substance. Therefore, this structural formula is not compatible with the name and manufacturing process reported for the substance.

Consequently, you shall provide more specific information on the manufacturing process of your substance, including the identity of the starting materials used, ratio of reactants, any relevant operating parameters (e.g. pH, parameters used to determine the completion of reaction, neutralization step) and a reaction scheme including all reaction and process steps.

Moreover, you shall ensure that the structural formula provided in section 1.1 is in line with the IUPAC name, the manufacturing process description and it is representative for your substance in terms of protonation/deprotonation of the ethylenediamine moiety.

Regarding how to report the manufacturing process description of the UVCB substance, this information shall be included in the "Description of the composition" field in section 1.2 of IUCLID. The structural formula shall be included in section 1.1 of IUCLID in the "Molecular and structural information" section.

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 cornerstone of all the REACH obligations.
In that respect according to chapter 4.3 of the Guidance, the following applies for UVCB substances:

- 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.
- Other constituents shall be identified as far as possible by a generic description of their chemical nature.
- For each constituent or group of constituents, the typical, minimum and maximum concentration levels shall be specified.

You have reported several groups of constituents in section 1.2. The first reported constituent [redacted] actually refers to two different constituents:

- specific iron complex [redacted]; and
- group of constituents "[redacted]"

In the description of analysis provided in section 1.4 in the document '[redacted] you state that "*according to the area ratio of the two peaks in the HPLC chromatogram ([redacted]% of peak1 [redacted]% of peak2) we assume that in our sample, the* [redacted]". Based on this information, the constituent [redacted]" present with a concentration above [redacted]% is reported together with a group of constituents ([redacted]) and from the analytical data report it is possible to verify that the two constituents are quantified separatly and could therefore be reported individually in section 1.2 of your dossier.

In addition, the name of the group of constituents ("[redacted]") is generic and no further information on the identity of the constituents covered by the group is provided, as well as no information on the specific condensation products that are covered by the group of constituents.

Furthermore, the constituent [redacted]" refers to an imine derivate. The imine derivate would not be an expected product of the described manufacturing process and the structural formula reported in section 1.1 with the remark "non specified (UVCB substance); structures given for the identified constituents" refer to a tertiary amine derivative. The identity of the constituent [redacted]" is therefore not consistent with the provided manufacturing process and structural formula.
You are accordingly requested to revise the composition information to:

- Report separately in section 1.2 of your dossier the constituents [redacted] and "[redacted]" and to provide the typical, minimum and maximum concentration levels for each of these constituents.
- Provide more details on the identity of the constituents covered by the group of constituents [redacted]) in terms of their chemical nature and plausible structure.
- Ensure that all reported constituents (in particular the constituent [redacted]) are consistent with the identifiers provided in section 1.1 and with the manufacturing process.

The revised composition information should be included in section 1.2 of IUCLID.

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

The description of analytical methods or appropriate bibliographical reference for the identification of the substance shall be sufficient to enable each substance to be identified. This means that the information included in the analytical report needs to enable understanding how the constituents required to be reported in the composition section of the IUCLID dossier have been identified and quantified.
You determined the content of constituents being iron chelated with Mannich base ligand by a HPLC method. The 2 peaks in the chromatogram ("[redacted]") were attributed to [redacted] and to "[redacted]". However, the chromatogram report is of low quality and the elution times and peak table are not readable.

In the results table (attachment "[redacted]) you state that "*Based on the molecular structure of* [redacted] *we assumed that in* [redacted] *one of the two Fe3+ is bonded only by one phenolic group instead of two, so to calculate the* [redacted] *contribution to the total absorption we applied a correction factor of (2/1.5)". and that "according to the area ratio of the two peaks in the HPLC chromatogram (*[redacted]*% of peak1 /* [redacted]*% of peak2) we assume that in our sample, the* [redacted]*% of the chelated iron is chelated as* [redacted] *and the* [redacted] *% as* [redacted]

[redacted]. *Considering the reaction conditions, we speculate that the two polycondensation products that we named* [redacted]*, are the most probable condensation products that could be present in our* [redacted] *samples.*"
However, no structural information on the condensation products is given and it is not clear how the two polycondensation products [redacted]) were identified.

The quantification of the substance is based on a chromatogram and peak table that are not fully legible and therefore cannot enable ECHA to verify the presence of the constituents of the substance.

In addition, this document also misses the necessary information to enable understanding the identity of the condensation products covered by the group of constituent "[redacted] reported in section 1.2.

Therefore ECHA concludes that the provided analytical information is not sufficient for establishing the composition of the registered substance and therefore its identity.

Therefore, you are requested to provide a readable chromatogram and peak table or the description of any other analytical method suitable to verify the composition of your substance. The description of the method shall be sufficient for the method to be reproduced.

Additionnally, you must provide information (e.g analytical method, assuptions based on chemical considerations and/or the manufacturing process) that allows to establish the identity of the condensations products.

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

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

An informal call with you was held on 23 March 2017, giving you the opportunity to revise substance identity issues. During the call you agreed to update your dossier addressing substance identity issues by 15 May 2017. As no update was received by the agreed deadline, ECHA contacted you by phone and agreed to extend the deadline to 7 September 2017. However, to date ECHA has not received your updated dossier.

The compliance check was initiated on 28 September 2017.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA did not receive any comments by the end of the commenting period.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

As no amendments were proposed, ECHA took the decision according to Article 51(3) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

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

2. Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.