ECHA
EUROPEAN CHEMICALS AGENCY

Helsinki, 25 October 2016

Addressee: [redacted]

Decision number: CCH-D-2114346784-40-01/F
Substance name: [hexane-1,6-diylbis[nitrilobis(methylene)]]tetrakisphosphonic acid, potassium salt
EC number: 254-135-7
CAS number: 38820-59-6
Registration number: [redacted]
Submission number: [redacted]
Submission date: 24.05.2013
Registered tonnage band: 100 to 1000 tonnes per year

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(s) in the IUPAC nomenclature or other international chemical name(s) (Annex VI, Section 2.1.1.);**
2. **Composition of the registered substance (Annex VI, Section 2.3.);**
3. **Description of the analytical methods (Annex VI, Section 2.3.7.).**

You may adapt the testing requested above according to the specific rules outlined in Annexes VI to X and/or according to the general rules contained in Annex XI of the REACH Regulation. In order to ensure compliance with the respective information requirement, any such adaptation will need to have a scientific justification, referring and conforming to the appropriate rules in the respective Annex, and an adequate and reliable documentation.

You are required to submit the requested information in an updated registration dossier by **1 February 2017**. You shall also update the chemical safety report, where relevant.

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

The scope of this compliance check decision is limited to the standard information requirement(s) of Annex VI, Section 2 of 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, shall 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 Hannu Braunschweiler, Head of Unit, Evaluation E1

[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

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(s) in the IUPAC nomenclature or other international chemical name(s) (Annex VI, Section 2.1.1.)

"Name or other identifier of the substance" is an information requirement as laid down in Annex VI, Section 2.1 of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

In line with chapter 4.2.1 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.3, February 2014) – referred to as "the Guidance" thereinafter, a mono-constituent substance is a well-defined substance with fully defined qualitative and quantitative composition that is named after the main constituent.

You identified the registered substance as a mono-constituent substance with generic EC and CAS identifiers and also with a generic molecular formula and generic IUPAC name "[redacted]".

All the provided identifiers refer to an entry for which the number of the potassium counter-ion is not defined and specified as "*x K*". Therefore these identifiers refer to all possible salts of the "[redacted]", hence potentially cover a group of substances. In fact, in section 1.2 of the technical dossier, eight different compositions referring to different salts of "[redacted]" are reported, as indicated in section 2 below.

The process description provided in section 3.1 of the technical dossier states that "[redacted]".

From the provided information, it is not clear whether you manufacture a single distinct substance with variation in the level of neutralisation of the phosphonic acid groups or whether the level of neutralisation is controlled yielding up to eight distinct substances. As a result, the information submitted in IUCLID section 1.1 does not allow ECHA to verify the identity of the registered substance as a well-defined mono-constituent substance.

Consequently, you are requested to revise the name and other identifiers of the registered substance, so it refers to a single substance to be covered by this registration.

Additionally, you should ensure that the name and identifiers used to describe the registered substance are chosen in accordance with the rules described in the Guidance.

If the substance is manufactured in such a way that the process (and in particular the neutralisation step) is not well-controlled and, as a consequence, the composition is highly variable and a specific salt cannot be isolated, the substance should be rather identified as a UVCB substance (Substance of Unknown or Variable composition, Complex reaction products or Biological materials). In such a case you would need to provide supporting documentation for why the registered substance is better identified as a UVCB rather than a well-defined substance.

In case that you decide 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) Regarding the chemical name, you should note that, for UVCB substances of such type as the substance that may be covered by this registration, ECHA considers that a chemical name is appropriate when it reflects the identity of the group of constituents present at ≥ 80% (w/w) or, if such a group does not exist, all the groups present at a concentration of ≥10% (w/w).
c) The description of the manufacturing process shall cover the identity and composition of the starting material used, ratio of the starting materials, steps and relevant process parameters. In addition you should note that for UVCB substances significant changes in the manufacturing processes may indicate multiple substances and consequently the requirement for multiple registrations. In particular, changes in the process leading to significant differences in the composition of the substance (such as changes leading to different salts of [redacted]") would be likely to lead to different substances that should be registered separately.

As for the reporting of the information in IUCLID, the chemical name and manufacturing process description shall be specified in the "IUPAC name" field and "Description" field in IUCLID section 1.1.

In case the current identifiers are not appropriate to describe the registered substance, you should 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, you should however indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "*The EC entry 254-135-7 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*". You should also specify, in the same "Remarks" field, any available and appropriate EC number for the substance. Any available CAS entry for the registered substance should be reported under the "CAS information" header of the reference substance in IUCLID section 1.1.

You should note that ECHA has established a process, 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.

Pending the resolution of the non-compliances addressed in the present decision, any possible adaptation of the identifier can only become effective once ECHA is in a position to establish unambiguously the identity of the substance intended to be covered by you with this registration. Should the information submitted by you as a result of the present decision enable ECHA to identify the substance unambiguously and result in a need to modify the identifier of the substance, the process of adapting the identifier will be considered relevant. In that case, ECHA will inform you in due time as to when and how the identifier adaptation process shall be initiated.

In any case, you should note that the application of the process of adapting the identifier does not affect your obligation to fulfil the requirements specified in this decision.

In the comments to the draft decision concerning name(s) in the IUPAC nomenclature or other international chemical name(s) (Annex VI, Section 2.1.1.) you agreed with ECHA that it is not correct to define the substance as a mono-constituent substance. You have proposed to identify the substance as a UVCB in section 1.1 of IUCLID dossier. Due to the fact that the substance is a substance with individual ionisable species, you have proposed to retain "x-salt identifiers" for the registered substance but indicated to improve the supporting information and compositional definition.

Irrespective of whether the newly provided information may be sufficient to meet the information requirement addressed in the decision, ECHA would like to highlight again the following:

- The naming of the substance should follow the naming convention for UVCB substances given in the Guidance for identification and naming of substances under REACH and CLP which is available on the ECHA website (http://www.echa.europa.eu/web/guest/guidance-documents/guidance-on-reach).
- If a specific composition (as referred to in your comments for Composition of the registered substance (Annex VI, Section 2.3.)) should be identified as a well-defined substance, you should consider your registration obligation to deliberate on whether or not these compositions should be regarded as substances in their own right and not being covered by the registration of the UVCB substance referred to in this decision.

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

"Composition of the substance" is an information requirement as laid down in Annex VI, Section 2.3 of the REACH Regulation.

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. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement. In that respect, according to the Guidance you shall note that, for well-defined substances, the following applies:

- Each main constituent (i.e. the constituent present at ≥80% for mono-constituent substance or each constituent present at ≥10% and <80% for multi-constituent substance) shall be identified and reported individually;

- Each impurity present at ≥1% or relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually;

- For each constituent, the typical, minimum and maximum concentration levels shall be specified regardless of the substance type.

According to the Guidance, chapter 4.2.2, a multi-constituent substance is a substance defined by its composition, for which more than one main constituent is present at a concentration ≥ 10% (w/w) and < 80% (w/w). To the contrary, a mono-constituent substance is a substance in which one constituent is present at a concentration of at least 80% (w/w) and which contains up to 20% (w/w) of impurities. Each constituent of a well-defined substance requires a complete chemical specification, including structural information. ECHA notes that you reported nine different compositions in section 1.2 of the IUCLID dossier. The first reported composition refers to an unspecified salt identified generically as [redacted] with the same reference substance as in section 1.1. The other eight compositions refer to individual salts identified respectively as mono-potassium, di-potassium, tri-potassium, tetra-potassium, penta-potassium, hexa-potassium, hepta-potassium and octa-potassium salt. Each of these salts is identified with the specific IUPAC, EC/list and CAS identifiers, which would indicate that up to eight distinct substances, are covered by this Registration, as also pointed out in section 1 hereinabove. Furthermore, the concentration range values for identified impurities with typical concentration above 1% are missing for all nine reported compositions.

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

You are requested to revise section 1.2 of your IUCLID dossier and to provide the missing information on the composition of the registered substance. You shall ensure that all reported compositions in the dossier refer to one and the same substance. All inconsistent compositional information shall be removed from the dossier. You shall also provide the typical, minimum and maximum concentration levels for each constituent, impurity and additive reported in section 1.2. The concentration range values must be representative for the registered substance as manufactured.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: You shall report individually any constituent or impurity required to be identified and specify at least one of the following identifiers: chemical name, CAS number, EC number and/or molecular formula, as well as the minimum, maximum and typical concentration, in the appropriate fields in Section 1.2 of the IUCLID dossier.

In the 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.

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.

In the comments to the draft decision concerning composition of the registered substance (Annex VI, Section 2.3.), you indicated your intention to update the composition information stating "according the information of the analytical reports, the substance will be renamed as an UVCB substance in an update" of the registration.

You agreed that the revision of the dossier is appropriate and propose to report the substance excluding any solvent which may be separated without affecting the stability of the substance or changing its composition. In addition you propose to report specific compositions of the product(s) as manufactured, stating the expected compositional range based on the different ionisation states present within relevant pH range(s). Classification and labelling relevant for each entry reported in section 1.2 will be presented in section 2.1.

Irrespective of whether the newly provided information may be sufficient to meet the information requirement addressed in the decision, ECHA would like to highlight again the following:

- If a specific composition should be identified as a well-defined substance according to the Guidance, you should consider your registration obligations under REACH and deliberate on whether or not these compositions should be regarded as substances in their own right and registered separately.

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

Annex VI, Section 2.3.7. of the REACH Regulation requires that each registration dossier contains a sufficiently detailed description of the analytical methods used for establishing the composition of the registered substance and therefore its identity. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

The registration dossier contains nine different compositions however only one set of analytical data was reported. The analytical data consist of the full set of spectral data (UV, IR, ^{1}H-NMR, ^{13}C-NMR and ^{31}P-NMR) and a quantification of different species. ^{31}P-NMR is used for quantification of the phosphorus containing constituents of the registered substance. A silver nitrate titration is used to quantify chlorides species. Anion and cation chromatography were also performed showing the presence of potassium and traces of sodium. The submitted ion chromatography used to quantify the potassium content gives a value of [redacted]% which is between the values expected for penta-potassium salt (x=5, theoretically [redacted]%) and hexa-potassium salt (x=6, theoretically [redacted]%).

However, the sample used for the analysis is only identified as "HMDTMP-xK" without any reference to the potassium content (x). It is therefore unclear whether the analyses have been performed on a sample of the specific substance which should be the subject of this registration.

The quantification of the phosphonate constituents was done at pH 5.4 by ^{31}P-NMR. However, as mentioned in the description of the manufacturing process, the distribution of the phosphonates constituents in the medium seems to be pH dependant ("[redacted]"). Consequently, it is unclear whether the analytical conditions used are appropriate to determine the composition of the substance. In addition, the calculations used to determine the concentration level of the different phosphonates required to be reported are missing from the registration dossier.

ECHA concludes on this basis that the description of the analytical methods is not detailed enough to allow verification of the reported results and confirm the identity and composition of the registered substance.

Therefore you are requested to provide a description of the analytical methods used for the identification and quantification of the constituents and impurities 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 calculations 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. You need to ensure that the composition reported in the dossier is consistent and fully supported by the description of the analytical methods used for the identification and quantification of the constituents and impurities required to be reported.

In the comments to the draft decision concerning description of the analytical methods (Annex VI, Section 2.3.7) you agreed that there is insufficient information describing the analytical methods used for establishing the composition of the substance. You propose to present a revised analytical report that summarises the evidence obtained by different analytical methods used to establish the composition of each manufactured / supplied product. You highlight in the supporting report the technical challenges foreseen when analysing the registered substance.

ECHA acknowledges the analytical complexity associated with the registered substance and would like to clarify that in case direct analytical determination of all constituents can be shown not to be feasible, an indirect determination with an appropriate justification may be acceptable. You may justify the use of indirect analytical methods by appropriate references to published literature references or by attaching the justification as an attachment to section 1.4 of the IUCLID dossier.

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.

The compliance check was initiated on 19 November 2015.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation:

ECHA notified you of the draft decision and invited you to provide comments. ECHA took into account your comments, which were sent within the commenting period, and they are reflected in the Reasons (Appendix 1).

ECHA notified the draft decision to the competent authorities of the Member States for proposal(s) for amendment(s).

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 request(s) in this decision, or to fulfil otherwise the information requirement(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.