EUROPEAN CHEMICALS AGENCY

Helsinki, 25 October 2016

Addressee: [redacted]

Decision number: CCH-D-2114343380-59-01/F
Substance name:
[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid, sodium salt
EC number: 244-751-4
CAS number: 22042-96-2
Registration number: [redacted]
Submission number: [redacted]
Submission date: 29.03.2011
Registered tonnage band: More than 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.) of the registered substance;**

2. **Composition of the substance (Annex VI, Section 2.3.) as explained in Appendix 1, Section 2; and**

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

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 sodium counter-ion is not defined and specified as "*x Na*". Therefore these identifiers refer to all possible salts of the "*[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid*", and hence potentially cover a group of substances. In fact, in section 1.2, 10 different compositions refering to different salts of "*[[(phosphonomethyl)imino]bis[(ethylenenitrilo) bis(methylene)]]tetrakisphosphonic acid*" are reported, as indicated in section 2 below.

Furthermore, in the chemical safety report attached to chapter 13, you state that the dossier covers a category of substances that consists of "[redacted]".

The process description provided in section 3.1 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 ten 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 well-defined mono-constituent substance. Consequently, you are requested to revise the name and other identifiers of the registered substance, so that it refers to 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 for identification and naming of substances under REACH and CLP (Version: 1.3, February 2014). The chemical name shall normally cover ≥ 80% (w/w) or, if such group does not exist, all the groups present at a concentration of ≥10% (w/w).
b) 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 "[[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphospho nic acid") would be likely to lead to different substances that should be registered separately.

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 244-751-4 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 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 you 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. You should ensure that the correct identifiers are used throughout the registration whenever reference to the specific substance which is subject of this registration is made.

You outlined in the comments to the draft decision how you intend to address the information requirement Name(s) in the IUPAC nomenclature or other international chemical name(s) (Annex VI Section, 2.1.1.) by providing two documents "[redacted]" and "[redacted]". In these documents, you have provided comments to the draft decision and provided information on how you intend to address the observation made by ECHA in relation to the process description provided in section 3.1. of the technical dossier. This is new information that has not been available earlier. Pending the submission of the information in the context of the not yet submitted updated dossier, ECHA can already point out the following:

- You provided information on a new description of the manufacturing process (for inclusion in section 3.1). This information does not include information on the ratio of the starting materials while this information is requested in the decision. The information eventually to be provided by you will be assessed on the basis of the updated dossier.
- In the new description of the manufacturing process, you have indicated that the target pH is in the range [redacted] (typically [redacted]) or in the range [redacted] (typically [redacted]). In document "[redacted]" you provided new information on the properties of different sodium salts of [[(phosphonomethyl)imino]bis [(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid. Based on the new information provided in the document "[redacted]", the two groups of commercial products where the target pH is [redacted]) or [redacted]) would have different compositions. For example at pH [redacted] only mono-, di- and tri- sodium salts would be present at concentrations [redacted]%, [redacted]%, and [redacted]% respectively (i.e. above 10%), while at pH [redacted] penta-, hexa- and heptasodium salts would be present at concentrations [redacted]%, [redacted]%, and [redacted]% respectively (i.e. above 10%). ECHA notes that in case all molecular species present are in equilibrium and variation between them is continuous, this variation may be described as a UCVB substance. In other cases it may be that there are partial salts with different compositions that should be registered separately. Therefore, you should ensure that the provided information on the manufacturing process refers to only one substance. Furthermore, you should ensure that the name and other identifiers of the registered substance refer to a single substance to be covered by this registration as requested in the decision.
- ECHA notes that the sentence "Therefore, if the different salts of "[[(phosphono methyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid are manufactured separately or isolated during the manufacturing process then they should be registered separately." on page 4 of the draft decision that was sent to you earlier during the compliance check process may be interpreted to restrict in an unintended way the options available to you with regards to the identification of the substance. Therefore, ECHA has amended the draft decision as outlined under above b).
- In document "[redacted]" you expressed your support for the document "[redacted]". You highlighted in that latter document a request for a meeting with ECHA to discuss the registration situation of all phosphonate salt substances, and for ECHA to examine all aspects and justifications provided in document "[redacted]". ECHA can already point out that the document "[redacted]" outlines potential consequences of a change of substance identity that are seen by (some of) the registrants. Furthermore, the document expresses the interest of (some of) the registrants in having a meeting with ECHA to gain assistance in reaching a solution.

In the document, (some of) the registrants also commit to improve the substance definition without delay, and if agreed to be necessary, to split the registration. ECHA notes that the information provided in document "[redacted]" relates to identification of phosphonate salt substances in general. ECHA acknowledges the initiative of (some of) the registrants to informally discuss the registration situation of all phosphonate salt substances with ECHA. However, ECHA notes that such discussions must be without prejudice to the present decision. Therefore, ECHA notes that the information to be provided by you will be assessed on the basis of the updated dossier.

2. Composition of the 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; and

- 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). In 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 speciation, including structural information.

ECHA notes that you reported eleven 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 10 compositions refer to individual salts identified respectively as mono-sodium, disodium, tri-sodium, tetra-sodium, penta-sodium, hexa-sodium, hepta-sodium, octa-sodium, nona-sodium and deca-sodium salt. Each of these salts is identified with the specific IUPAC, EC/list and CAS identifiers, which would indicate that up to ten 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 11 reported compositions. In addition, ECHA points out that one of the impurities identified generically as "[redacted]", containing three phosphonomethyl substituents at variable positions, is present at a typical concentration of 10% in all compositions. Based on the ^{31}P-NMR analysis this entry covers a group of three different impurities that have been quantified and identified separately (present at [redacted]%, [redacted]%, and [redacted]%). However, these impurities are not reported individually in the composition, as required in line with the Guidance.

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 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.

You outlined in the comments to the draft decision how you intend to address the information requirement "Composition of the substance" (Annex VI, 2.3.) by providing two documents "[redacted]" and "[redacted]". In these documents, you have provided comments to the draft decision and new information that has not been available earlier. Irrespective of whether the newly provided information in the updated dossier may be sufficient to meet the information requirement addressed in this decision, ECHA can already point out the following:

- In document "[redacted]" you provided information, including minimum and maximum concentration levels of the constituent(s) and impurities, on the composition of the acid that is used as a starting material for the manufacturing of your substance. The provided information would seem to be in line with the expectations in the decision regarding the missing information on the impurities that need to be reported individually in the composition. However, the information to be provided by you will be assessed on the basis of the updated dossier.

- In document "[redacted]" you provided new information on the properties of different sodium salts of [[(phosphonomethyl) imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid. The provided information indicates that the composition of the substance depends on the target pH (i.e. the degree of neutralisation), because at any specific pH, multiple individual sodium salts are present (e.g. mono-, di-, and trisodium salts of [[(phosphonomethyl)imino]bis[(ethylenenitrilo)bis(methylene)]]tetrakisphosphonic acid). Based on the new information provided in the document "[redacted]", the two groups of commercial products where the target pH is [redacted] (typically [redacted]) or [redacted] (typically [redacted]) would have different compositions. For example at pH [redacted] only mono-, di- and tri- sodium salts would be present at concentrations [redacted]%, [redacted]%, and [redacted]% respectively (i.e. above 10%), while at pH [redacted] penta-, hexa- and heptasodium salts would be present at concentrations [redacted]%, [redacted]%, and [redacted]% respectively (i.e. above 10%). ECHA notes that in case all molecular species present are in equilibrium and variation between them is continuous, this variation may be described as a UCVB substance. In other cases it may be that there are partial salts with different compositions that should be registered separately. Therefore, you should ensure that all reported compositions in the dossier refer to one and the same substance.
- In document "[redacted]" you indicated that you will update section 1.2 of the IUCLID dossier as soon as an agreement with ECHA and the SIEF is reached regarding how to submit the composition of the substance. ECHA notes that any discussions between ECHA and the SIEF must be without prejudice to the present decision. Therefore, ECHA notes that the information to be provided by you will be assessed on the basis of the updated dossier.

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 method 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 eleven differents compositions. However only two different sets of analytical data respectively for the compositions referring to the disodium salt and to the heptasodium salt were provided. Both sets of data consist of spectral data such as infra-red (IR), ultra-violet (UV)/visible; nuclear magnetic ressonance (NMR) spectra and ion chromatography techniques that were used for the quantification of the constituents and impurities present in the substance. For both salts, the quantification of the organic part of the main constituent is based on ^{31}P-NMR and the content of "sodium" is determined by ion chromatography.

However it is unclear how exactly the quantification has been done as the calculations used to determine the substance purity and to support the composition recorded in IUCLID section 1.2 are missing from the registration dossier. In addition, as mentioned in the description of the manufacturing process, provided in IUCLID section 3.1 "[redacted], the distribution of the phosphonates constituents seems to be pH-dependant. However, you indicated that the quantification of the phosphonates constituents is carried out by ^{31}P-NMR run at fixed pH 5.4 for both salts.

Therefore, it is unclear whether the analytical conditions used are appropriate to determine the purity of the specific substance.

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 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. 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, 2.3.7.), you indicated your intention to update the analytical information.

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 2 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 and did not amend the requests.

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

3. In relation to the information required by the present decision, the sample of substance used for the new test(s) must be suitable for use by all the joint registrants. Hence, the sample should have a composition that is range of substance composition manufactured or imported by the joint registrants. It is the responsibility of all joint registrants who manufacture or import the same substance to agree on the appropriate composition of the test material and to document the necessary information on their substance composition. In addition, it is important to ensure that the particular sample of substance tested in the new test(s) is appropriate to assess the properties of the registered substance, taking into account any variation in the composition of the technical grade of the substance as actually manufactured or imported by each registrant. If the registration of the substance by any registrant covers different grades, the sample used for the new test(s) must be suitable to assess these grades. Finally there must be adequate information on substance identity for the sample tested and the grade(s) registered to enable the relevance of the test(s) to be assessed.