ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114306547-50-01/F Helsinki, 7 August 2015

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

For orthoboric acid, compound with 2,2'-iminodiethanol, CAS No 67952-33-4 (EC No 267-886-0), 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 orthoboric acid, compound with 2,2'-iminodiethanol, CAS No 67952-33-4 (EC No 267-886-0), 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 100 to 1000 tonnes per year. This decision does not take into account any updates after the deadline for updating (15 March 2015) communicated to the Registrant by ECHA on 6 February 2015.

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 11 June 2014.

On 12 November 2014 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision. That draft decision was based on submission number [redacted].

By 19 December 2014 the Registrant did not provide any comments on the draft decision to ECHA.

On 18 December 2014 the Registrant updated his registration with the submission number [redacted].

The ECHA Secretariat considered the Registrant's update.

The information is reflected in the Statement of Reasons (Section III) whereas no amendments to the Information Required (Section II) were made.

On 11 June 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

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. 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 **16 November 2015** an update of the registration dossier containing the information required by this decision.

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.

A. 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, 2.1.)

ECHA notes that the Registrant identified the registered substance as of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). The naming of UVCB substances shall consist of two parts: the chemical name and the more detailed description of the manufacturing process. According to the ECHA "Guidance for the identification and naming of substances under REACH and CLP" (Version: 1.3, February 2014), UVCB substances cannot be sufficiently identified by their chemical composition and the main identifier for UVCB substances is the description of the manufacturing process, including final or most relevant steps of the processing. ECHA notes that the registration does not contain the required details on the manufacturing process, that would enable the identification of the registered UVCB substance.

In the initial dossier no description of the substance and of the manufacturing process was provided in section 1.1 and the description included in section 3.1 was not sufficiently detailed as it did not contain information on the ratio(s) of starting materials used, process

steps and process parameters. This information is considered as a key element to establish the identity of the registered substance. In addition, the EC and CAS entries (267-886-0 and 67952-33-4, respectively) and the molecular formula provided in section 1.1 (C4H11NO2.xBH3O3) did not define the boric acid /amine ratio and its variability. Furthermore, in the part B of the CSR ("IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES") attached in section 13 the Registrant indicated that the composition may vary, and provided also other EC and CAS identifiers for the registered substance: "*DEA Polyborate is a UVCB. The substance identified by (amongst others) the following CAS and EC identifiers represent a range of compositions, all broadly similar, but each does not give the extent of the variation of the molecules in the complex variable system.*
EINECS Name (EC no; CAS no): Boric acid (H3BO3), reaction products with diethanolamine (290-817-0; 90268-17-0) orthoboric acid, compound with 2,2'-iminodiethanol (267-886-0; 67952-33-4) Boric acid, compd. with 2,2'-iminobis[ethanol] (270-366-6; 68425-66-1 Boric acid, reaction products with diethanolamine (273-238-8; 68954-07-4)". These additional EC/CAS entries provided in the CSR also do not define the ratio of reactants and its variability.

The ratio of these reactants may be however a significant parameter that can strongly affect the composition and therefore identity of the registered substance.

In the initial draft decision sent to the Registrant for comments, the Registrant was reminded that if the substance covered by the registration is manufactured according to different manufacturing processes, including the use of different ratios of reactants or process parameters, then the detailed description of the manufacturing process required hereinabove shall be reported separately for each manufacturing process. A manufacturing process may be different when the processing steps and/or processing parameters affecting the identity of the substance, are different.

The Registrant shall note that any significant change in the manufacturing process or source would lead to different UVCB substances which shall be registered separately. It is the responsibility of the registrant to ensure that the dossier refers to one substance and that the identity of this substance is verifiable based on the information included in section 1.1 of the IUCLID dossier.

After the receipt of the draft decision the Registrant updated the dossierand provided a more detailed description of the manufacturing process, including information on the temperature and ratio of the reactants used. More specifically the Registrant explained that "[redacted])". ECHA notes, however, that there is inconsistent, with the above, information in the CSR (References) suggesting that different ratios of the starting materials can be used (i.e. not only [redacted] but also [redacted]). Such change in the ratio of reactants from [redacted] to [redacted], in the absence of any justification provided, may be regarded as a significant process parameter.

However, the chemical /IUPAC name of the registered substance "orthoboric acid, compound with 2,2'-iminodiethanol", the EC /CAS identifiers and molecular formula (C4H11NO2.xBH3O3) provided in the updated dossier are still overly generic and they do not specify the ratio of the boric acid to amine that is used by the Registrant.

The identifiers currently used (the chemical /IUPAC name, CAS, EC, molecular formula) are therefore overly generic and inconsistent with the description of the manufacturing process,

as they cover any ratio of the reactants (including [redacted], [redacted] and any other), which may lead to different compositions, hence potentially different substances.

In line with the above, the Registrant is requested to revise the identifiers of the registered substance including the chemical name and the molecular formula in order to reflect the ratio of the reactants used.

Regarding how to report the requested information in IUCLID the following applies:

- The revised chemical name shall be included in the IUPAC name field in Section 1.1 of the IUCLID dossier and CSR.
- The revised molecular and structural formula and other identifiers shall be included in their respective fields in Section 1.1 of the IUCLID dossier and CSR.
    - The relevant appropriate CAS entry shall be included in the "CAS information" field, if available. Where the current CAS entry (CAS number 67952-33-4 and CAS name Boric acid (H3BO3), compd. with 2,2'-iminobis[ethanol]) does not identify the registered substance, it shall be reported under the "Related CAS information" header in IUCLID Section 1.1 . Similarly where the current EC entry does not correctly identify the registered substance, it will need to be revised. For technical reasons the Registrant is requested at this stage, not to remove or revise the EC entry in the updated dossier. As this registration is linked to this EC entry in REACH-IT, the IT system will not accept the updated dossier as an update when the EC entry has changed. The Registrant shall instead include the following in the "Remarks field" of the reference substance: "This EC entry is not appropriate to identify the registered substance. This identifier cannot be modified in the present registration at this stage for technical reasons."

The Registrant shall ensure consistency of the substance identity information provided in the dossier (including CSR).

Further information on how to report the chemical name, the molecular and structural formula, other identifiers and the description of the manufacturing process is available in "Data Submission Manual Part 18 - How to report the substance identity in IUCLID 5 for registration under REACH" published on the ECHA website at http://echa.europa.eu/web/guest/support/dossier-submission-tools/reach-it/data-submission-industry-user-manuals.

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 corner stone of all the REACH obligations.

ECHA notes that the registration does not contain sufficient 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, in section 1.2 of the initial dossier, the Registrant provided the same reference substance as in section 1.1 with purity of [redacted]%. In the remarks field of the reference substance in section 1.2 of the IUCLID dossier, the Registrant provided information indicating that different constituents are however present in the registered substance: "*DEA polyborates are complex mixtures of (HO(CH2)2)2NH2+ salts, borate esters, structures where the free electrons of the NH imino moiety takes part in cyclisation and various polyborates, all existing in rapid equilibrium*". Furthermore it was indicated in the CSR part B, that for the registered substance "*Whenever boric acid is dissolved in an*

alcohol or an alcoholic water mixture at neutral or alkaline pH, a substantial portion of the resulting solution consists of borate esters (also known as boresters or alkoxyboranes (IUPAC). These are esters of the type (HO)2BOR, HOB(OR)2, and B(OR)3, where R is an alcohol, alcoholamine etc". However, the relevant individual constituents or groups of constituents have not been identified and reported in IUCLID section 1.2.

In the updated dossier, the Registrant has revised the composition of the registered substance reporting 3 groups of constituents and water in section 1.2. These 3 groups seem to refer to theoretical constituents that can be formed during the manufacturing process: "Ester reaction products of diethanolamine and boric acid", "Polyborates of Diethanolamine and Boric acid" and "Aminium salts of diethanolamine and boric acid" correspondingly. However, this information is not supported by the analytical data attached in section 1.4. Furthermore, it is unclear how the broad concentration ranges ([redacted]%) for the 3 groups of constituents were established. It is also unclear whether the composition in the updated dossier was derived from any analytical data or it is rather theorethetical composition (e.g. based on the knowledge of the starting materials, reaction stoichiometry, equilibrium data or chemistry of borate systems). If it is the latter then the detailed explanation is needed on how the theorethetical composition, including concentrations, has been derived.

Furthermore, the description of the manufacturing process provided in the updated dossier may suggest that different compositional grades may be manufactured (because there is variation in the molar ratio of starting materials from [redacted] to [redacted]) as it is indicated above, however the Registrant did not report separately these compositions in section 1.2 of the dossier.

The Registrant should note that for UVCB substances such as the registered substance, the following applies:

- 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 for ECHA to establish the composition of the substance as manufactured and to use the compositional information as one identifier for the registered substance.

For each constituent and group of constituents, the typical, lower and upper concentration levels shall be indicated. The concentration values shall be representative for the manufactured substance. The fact that constituents exist in fast equilibrium does not prevent the Registrant to provide representative information on the overall composition of the registered substance.

It should also be noted that any quantity of solvent which can be removed without irreversible changes in the (dynamic) composition upon re-addition of the solvent, regardless of whether a shift in the initially existing equilibrium between the constituents takes place upon that removal, shall not be included in the substance composition.

If the actual composition of the registered substance cannot be derived due to the complexity and/or technical limitation of the analytical methods, the Registrant shall provide robust scientific justification including analytical evidence and/or bibliographic references supporting this justification (as explained also later in section III b, see below). Nevertheless at least the theoretical composition derived on the basis of the knowledge of

the starting materials, reaction stoichiometry and the chemistry of similar borate systems shall be provided in IUCLID section 1.2.

In line with the above, the Registrant is requested to provide any information which is suitable and necessary to allow ECHA to establish and verify the composition and the name of the registered substance.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: the Registrant shall report the composition of the registered substance in IUCLID Section 1.2. 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, shall be provided in the appropriate fields in IUCLID. For the other constituents that can 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, shall be provided in the appropriate fields in IUCLID.

Where the Registrant covers different grades of the same substance in a registratiothe Registrant shall report separately the compositional information of each grade. In practice if the substance covered by the registration has two (or more) different compositions, these must be presented separately.

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) on the ECHA website.

3. The description of the analytical methods (Annex VI, 2.3.7.)

ECHA notes that the Registrant has not provided a sufficient description of the analytical method used for the identification and quantification of the registered substance including its constituents as required by Annex VI, 2.3.7. of the REACH Regulation.

More specifically, the Registrant provided results of NMR, IR, UV and an elemental analysis for C, N and B content in the initial dossier. However description of these methods do not allow unambigous identification of constituents /groups of constituents that may be present in the registered substance, as it is indicated in the Registrant's remarks in section 1.2 of the IUCLID dossier and in the CSR. Furthermore no quantitative analysis of the substance that would determine content of constituents /groups of constituents has been provided in the dossier.

The Registrant has provided justification for the absence of HPLC analysis that can be followed by ECHA. However, ECHA notes that when a direct analysis is not possible, other alternative analytical methods may be applied (including these based on the derivatization or using model systems) to analyze the composition of the registered substance.

The Registrant provided the same set of analytical data in the updated dossier. This analytical data does not support the composition of the registered substance as it is indicated in section III. A. 2 hereinabove.

Therefore, the Registrant is requested to submit the missing information on the description of the analytical method(s) used for the identification and quantification of the registered substance including its composition. The description shall be sufficient for the methods to be reproduced and shall therefore include details of the experimental protocol followed, any

calculation(s) made and the results obtained. The results of quantitative analysis shall be recorded for the manufactured substance.

Should a certain method not be applied due to a technical limitation, the Registrant shall provide robust scientific justification including analytical proof and/or bibliographic references supporting this justification. In case when the reported composition is based on theoretical assumptions or calculations, all information that is necessary to understand how this composition has been estabilished need also to be provided in section 1.4.

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

The Registrant is reminded that this decision does not take into account any updates submitted after 12 March 2015. All the new information in the later update(s) of the registration dossier will however be assessed for compliance with the REACH requirements in the follow-up evaluation pursuant to Article 42 of the REACH Regulation.

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 Leena Ylä-Mononen, Director of Evaluation

[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.