EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114315468-47-01/F Helsinki, 16 February 2016

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

For Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts, EC No 291-454-0 (CAS No 90411-76-0), 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 Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts, CAS No 90411-76-0 (EC No 291-454-0), 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 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 05 May 2015.

ECHA notified the Registrant of the draft decision on 12 May 2015 and invited the Registrant to provide comments.

ECHA received the Registrant's comments on the draft decision on 18 June 2015.
The ECHA Secretariat considered the Registrant's comments. As a result, ECHA did not amended the information required in the draft decision.

On 29 October 2015, ECHA notified the competent authorities of the Member States of its draft decision and invited them to propose amendments to the draft decision under Article 51 of the REACH Regulation.

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

EUROPEAN CHEMICALS AGENCY

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, molecular and structural formula or other identifiers of the substance (Annex VI, 2.1 and 2.2)
2. Composition of each substance (Annex VI Section 2.3 of the REACH Regulation).
3. Spectral data (Annex VI Section 2.3.5 of the REACH Regulation).
4. Description of the analytical methods (Annex VI Section 2.3.7 of the REACH Regulation).

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 **23 May 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.

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, molecular and structural formula or other identifiers of the substance (Annex VI, 2.1 and 2.2)

ECHA notes that the Registrant has not provided sufficient information to identify the substance, as required by Annex VI, Section 2.1 of the REACH Regulation. Based on the information included in Section 1.1 of the dossier, it is not possible to unambiguously establish the identity of the substance registered.

More specifically, 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 such as the registered substance shall consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process (including details on the starting materials), as indicated in chapter 4.3 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.3, February 2014) - referred to as "the Guidance" thereinafter. ECHA observes that the identifiers of the substance provided by the Registrant in IUCLID section 1.1 are generic and inconsistent and that the Registrant did not provide sufficient information on the manufacturing process.

ECHA notes that the information provided in the dossier regarding the identifiers of the substance is generic and inconsistent:

- The chemical name, EC and CAS entries refer to a UVCB substance identified as "*Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts*". The name associated to these entries is based on the reaction process. However it is overly generic and can potentially cover several sodium salt substances, each with different levels of sulfonation from the reaction products of different ratios of aniline and nitrobenzene under different reaction conditions. In addition, the EC and CAS entries reported for the registered substance are not associated with any specific structural formula that would clarify the identity of the substance intended to be covered by these entries.

- The reported structural formula refers to a more specific chemical structure in contrast to the very broad structures possible under the EC and CAS entries. However, the reported structure is generic and does not provide sufficient information about the constituents of the substance. In particular, the structural formula suggests the registered substance being based on constituents that have a sequence of quinoxaline moieties with variable number. However no information on the sequence number variation is provided. In addition, the reported structure is not consistent with the sodium salt substance described by the reported EC and CAS entries because it does not include sodium as the counter ion.

- The reported name in the IUPAC name field ("[redacted]") is also overly generic. The name represents a class of organic dyes and can cover a large number of different substances.

ECHA also notes that a description of the manufacturing process was provided in IUCLID section 3.1. The Registrant reported that the substance is produced by a "[redacted]". However, the description is not sufficiently detailed to enable the identity of the substance to be verified. In particular, details on the ratio of the starting materials and on the reaction conditions are missing from the description. ECHA considers that the ratio of the starting materials and the reaction conditions are essential factors determining the composition a substance, and therefore necessary for the identification of the registered substance.

As a consequence, the identifiers reported in section 1.1 and the description of the manufacturing process described in section 3.1 of the IUCLID dossier are not sufficient for the identification of the registered substance.

In line with Annex VI, Sections 2.1 and 2.2 the Registrant is requested to revise the name, molecular formula and other identifiers so that the registration unambiguously identifies the substance registered.

Concerning the description of the manufacturing process, this description shall be sufficiently detailed to allow ECHA to understand which starting materials are used, and how any other steps and process parameters may affect the substance composition and therefore its identity.

Where the Registrant covers different grades of the substance in a registration, the Registrant shall report separately the source and manufacturing process of each grade. ECHA highlights that grades for which a manufacturing process description is not provided may eventually not be considered being covered by the registration.

The Registrant shall ensure that the information reported is consistent throughout the dossier.

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

- The revised IUPAC name shall be reported in the IUPAC name fiels in IUCLID section 1.1.
- The revised structural information shall be reported in the the appropriate IUCLID fields in Section 1.1.
- The relevant appropriate CAS entry shall be included in the "CAS information" field, if available. Should a reported CAS number not be specific but related to the registered substance, it may be reported under the "Related CAS information" header in IUCLID section 1.1.
- Regarding how to revise the EC entry, 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. To revise the EC entry the Registrant shall indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 291-454-0 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". The Registrant shall also specify, in the same "Remarks" field, any available and appropriate EC number for the substance. In addition, the Registrant shall note that ECHA has established processes, subject to certain conditions, enabling registrants to adapt the EC/list identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned. Should a Registrant 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 for a possible adaptation of the registration.
- Regarding how to report the description of the UVCB substance, the information shall be included in the Description field in IUCLID section 1.1.

Further technical details on how to report the identifiers of UVCB substances in IUCLID are available in paragraph 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.

The Registrant outlined in the comments to the draft decision how he intends to address the information requirement concerning name or other identifier of the substance (Annex VI, 2.1.):

- EC name:

The Registrant indicated that the new analytical results will most probably not be satisfactory to define a more accurate EC name and suggests *"to keep the EC name "Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts" in connection with a specific description of the technological process"*.

ECHA notes that new analytical results might be valuable to define a more accurate EC name; however in the absence of useful analytical results other information can be taken into consideration to define the name of the substance (e.g specific identity of the starting materials). Additionally, ECHA points out that the description of the technological process is part of the naming of a UVCB, but it does not substitute the request to provide an accurate name to identify the registered substance.

- Structural formula:

The Registrant indicated is intention to update the structural formula *"on the basis of new analytical results and all available data".*

- IUPAC name:

The Registrant indicated is intention to update the IUPAC name in case new analytical results are obtained.

As for the EC name, ECHA notes that new analytical results might be useful to define an accurate IUPAC name; however in the absence of suitable analytical results other information can be taken into consideration to define the IUPAC name (e.g specific identity of the starting materials).

- Grades of the substance:

The Registrant states in his comments that the registration covers only one grade, and explains that "[redacted]".

ECHA points out that this description only explains that the substance is the same in both aqueous and solid forms. To verify whether the registration covers only one grade more details on the description of the manufacturing process are necessary to be provided (e.g starting materials, processes used and related parameters) showing that only one grade of the substance is manufactured.

2. Composition of each substance (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 cornerstone of all the REACH obligations. ECHA notes that the Registrant has not included sufficient information on the composition of the substance to enable the identity of the registered substance to be verified, as required under Annex VI, Section 2.3. of the REACH Regulation.

ECHA notes that one generic reference substance covering most of the constituents of the UVCB substance (*"Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts"*) is reported as the main constituent and three other constituents ([redacted]) are reported as impurities in the IUCLID section 1.2.

The reported group of constituents has the same identity as reported for the registered substance in IUCLID section 1.1. The information provided for this group of constituents is not sufficiently detailed to determine the identities of the constituents that are intended to be covered by this generic group.

According to chapter 4.3 of the Guidance, for reporting the composition of a 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.

For each constituent and group of constituents, the minimum, maximum and typical concentration shall be reported.

In line with Annex VI Section 2.3, the Registrant is required to revise the composition to include sufficient information on the identities of the constituents and/or group of constituents covered by the Registration. In particular, the registrant shall provide more details on the variability of the quinoxaline moieties in the generic group of constituents "Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts".

In addition, the Registrant shall note that, for UVCB substances such as the registered substance, due to the complexity of the composition, the terms "main constituents" and "impurities" are not regarded as relevant, and therefore the composition breakdown shall be entirely reported under "constituents".

The Registrant shall ensure that the information reported is consistent throughout the dossier.

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.

Where the Registrant covers different grades of the same substance in a registration, the Registrant shall report separately the compositional information of each grade. This means that if the substance covered by the registration has two (or more) different compositions, then these must be presented separately. Corresponding analytical data to enable the identity and composition of each grade listed in 1.2 to be verified shall be included in Section 1.4. Information on how to report several compositions in IUCLID is specified in paragraph 2.3, Q&A 8 of the "Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH".

ECHA highlights that failure to report separately the compositional information of each grade of a substance may result in one or more grades not being covered by this registration.

In the comments to the draft decision concerning the composition of the substance (Annex VI, 2.3.), the Registrant indicated his intention to update the composition information based on new analytical results.

3. Spectral data (Annex VI Section 2.3.5 of the REACH Regulation).

"Spectral data" is an information requirement as laid down in Annex VI, Section 2.3.5. of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the registration does not contain any Nuclear Magnetic Resonance (NMR) or Mass spectrum (MS) which is required according to Annex VI Section 2.3.5. of the REACH Regulation to support the identity of the registered substance. Instead the Registrant provided a justification for not providing this information ("*Conducting is technically not possible, as the* substance is an UVCB substance and per NMR not determinable"). ECHA agrees that due to the UVCB nature of the substance, the NMR spectrum will probably not give sufficient information to fully verify the identity of the substance. However, NMR spectroscopic analyses such as a ^{1}H-NMR or a ^{13}C-NMR are powerful tools for structure characterisation and elucidation due to characteristic chemical shifts and spin-spin coupling

which also reflect the relative abundance of individual atoms. As all reported constituents contain characteristic hydrogen and carbon atoms, NMR is an appropriate analytical method to characterise the substance.

Therefore, in line with Annex VI, Section 2.3.5, the Registrant is requested to submit a NMR spectrum such as a 1H-NMR or a 13C-NMR or a mass spectrum including the corresponding interpretation of the fragmentation scheme.

The Registrant shall ensure that the reported information is consistent throughout the dossier.

Regarding how to report the requested information in IUCLID, the spectra should be attached in IUCLID section 1.4.

In the comments to the draft decision concerning the spectral data (Annex VI, Section 2.3.5), the Registrant indicated his intention to update the registration dossier with a ^{1}H-NMR spectrum.

4. Description of the analytical methods (Annex VI, Section 2.3.7 of the REACH Regulation).

ECHA notes that the Registrant has not provided sufficient information on the methods used to determine the identity and composition of the substance registered by his legal entity, as required by Annex VI, 2.3.7. of the REACH Regulation. ECHA observes that the Registrant did not provide sufficient description of the analytical methods used for the identification and quantification of the constituents and/or groups of constituents required to be reported in the composition of the registered substance.

More specifically, ECHA notes that the Registrant provided an analytical report [redacted] in section 1.4 of the IUCLID dossier. However, the reported method only quantifies [redacted] (minor constituent of the substance) and therefore, does not provide sufficient information to properly quantify all the constituents of the substance.

In addition, the quantification of the generic group ("*Hydrochloric acid, reaction products with aniline and nitrobenzene, sulfonated, sodium salts*") was estimated by back-calculation (subtracting the quantified [redacted]). This type of quantification is not considered accurate as the determination of the composition is not based on the identities of the constituents. The Registrant shall note that ECHA considers that an accurate quantification of the substance can only be obtained by a direct quantification method of the constituents.

As a result, the analytical data reported by the Registrant does not provide sufficient information regarding the quantification of all the constituents of the substance and does not enanble the identity of the substance to be verified.

In line with Annex VI Section 2.3.7 the Registrant is requested to submit a suitable description of the analytical methods (chromatography or any other suitable analytical method) used for the identification and quantification of the constituents and groups of constituents 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.

The Registrant shall ensure that the reported information is consistent throughout the dossier.

Regarding how to report the requested information in IUCLID, the information should be attached in IUCLID section 1.4.

In the comments to the draft decision concerning the description of the analytical methods (Annex VI, 2.3.7), the Registrant indicated his intention to update the registration dossier by stating that *"The Registrant intends to submit reports of all additional testings in a dossier update. These reports will also state any experiment which were undertaken but failed."*

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 Guilhem de Seze, 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.