

Decision number: CCH-D-2114289048-40-01/F

Helsinki, 21 November 2014

**DECISION ON A COMPLIANCE CHECK OF A REGISTRATION PURSUANT TO ARTICLE 41(3) OF REGULATION (EC) NO 1907/2006****For Aluminum chloride, basic, CAS No 1327-41-9 (EC No 215-477-2), 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 Aluminum chloride, basic, CAS No 1327-41-9 (EC No 215-477-2), submitted by [REDACTED] (Registrant). The scope of this compliance check 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 1000 tonnes or more per year. This decision does not take into account any updates submitted after 4 September 2014, the date upon which ECHA notified its draft decision to the Competent Authorities of the Member States pursuant to Article 51(1) of the REACH Regulation.

The substance subject to the present decision is provisionally listed in the Community rolling action plan (CoRAP) for start of substance evaluation in 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 13 November 2013.

On 11 April 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].

On 22 May 2014 ECHA received comments from the Registrant on the draft decision.

On 17 July 2014 the Registrant updated his registration dossier with the submission number [REDACTED].

The ECHA Secretariat considered the Registrant's comments and update. The information is reflected in the Statement of Reasons (Section III) whereas no amendments to the Information Required (Section II) were made.

On 4 September 2014 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

### **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:

- A. Name, molecular and structural formula or other identifier of the substance (Annex VI, 2.1 and 2.2): Information which is suitable and necessary to allow ECHA to establish and verify the name and the identity of the registered substance, as specified under section III.A.1 below;
- B. Composition of the substance (Annex VI, 2.3): Information which is suitable and necessary to allow ECHA to establish and verify the composition and the identity of the registered substance, as specified under section III.A.2 below;
- C. The description of the analytical methods (Annex VI section 2.3.7.), as specified under section III.A.3 below.

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated registration to ECHA by **2 March 2015**.

## III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein does not comply with the requirements of Article 10 of the REACH Regulation and Annex VI thereof. Consequently, the Registrant is requested to submit the information mentioned above that is 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 and 2.2 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

Initially, the Registrant identified the registered substance as a well-defined mono-constituent substance and provided in section 1.1 of the initial dossier ambiguous identifiers which referred to more than one substance. In the updated dossier, the Registrant has changed the substance type to a UVCB substance (a substance of Unknown or Variable composition, Complex reaction products or Biological materials).

In accordance with chapter 4.3 of the "Guidance for identification and naming of substances under REACH" (Version: 1.3, February 2014), referred to as the Guidance thereafter, the naming of a UVCB substance consists of two parts: the chemical name and the more detailed description of the manufacturing process. Therefore, correct information on the chemical name, allowing an unambiguous identification of the registered substance, is required to be provided for a UVCB substance. Furthermore, accurate information on the structural formula of the substance is necessary for ECHA to enable the identity of the registered substance to be verified.

In Section 1.1 of the updated registration dossier the Registrant has identified the substance with the EC and CAS entries corresponding to "Aluminium chloride, basic" (EC no. 215-477-2 and CAS no. 1327-41-9). The molecular formula reported in section 1.1 has been revised to " $Al(OH)_x(Cl)_{(3-x)}$ , with  $x$  ranging from [REDACTED] and typically being [REDACTED]", which corresponds as well to the basic aluminium chloride (i.e. aluminium hydroxy chloride) and is in line with the identification of the substance as a UVCB. In section 3.1 the Registrant has given sufficient details on their own manufacturing process as is required to be provided for a UVCB substance. However, the Registrant has kept in the IUPAC name field the chemical name "aluminium trichloride" which was also provided initially. In addition, the structural information (structural formula and InChI) included in section 1.1 also refers to "aluminium trichloride".

The Registrant is reminded that aluminium trichloride,  $AlCl_3$  (with its own EC number: 231-208-1; CAS number: 7446-70-0) is a different substance from basic aluminium chloride. Therefore, the chemical name and the structural information provided in section 1.1 are not in line with the EC and CAS entries and the molecular formula provided for the registered substance.

In his comments to the draft decision, the Registrant indicated that the substance covered by the registration corresponds to the basic aluminium chloride, and not the pure  $AlCl_3$ . ECHA takes note of this comment and concludes that the currently provided chemical name and structural information do not correspond to basic aluminium chloride .

Accordingly, the Registrant is requested to revise the chemical name and the structural formula of the substance such that they are representative of the registered substance and allow ECHA to unambiguously identify the registered substance.

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.
- The revised structural formula and InChi code (if available) shall be included in their respective fields in Section 1.1 of the IUCLID dossier.

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 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.

Initially, the Registrant reported one composition in Section 1.2 of the dossier and this composition identified its main constituent with the same generic reference substance as in section 1.1 "Aluminum chloride, basic". From this limited information and due to the inconsistencies in the identifiers which were reported in Section III.A.1 of the draft decision, the composition of the substance manufactured/imported could not be established on the basis of the initial information.

In the updated dossier, the Registrant has reported one composition block named as "Aluminium chloride, basic - Medium OH/Al ratio". This composition includes two constituents: water and one generic group of constituents "Aluminium (hydroxy) chloride complexes / Polyaluminium Chloride", with the remark that "Substance is manufactured and supplied only as aqueous solution".

ECHA observes that the Registrant did not provide sufficient and appropriate information to allow the composition of the registered substance to be verified, as explained under points (i) and (ii) below.

### (i) Inclusion of water in the composition

ECHA considers that the information in the dossier does not allow ECHA to confirm that the water included in the updated composition shall be considered as part of the registered substance. According to the information in the dossier it appears that the water shall rather be regarded as a solvent which is not part of the registered substance.

Article 3(1) of the REACH Regulation specifies that a substance shall not include a solvent which may be separated without affecting the stability of the substance or changing its composition.

Although the Registrant indicates that the substance is manufactured as an aqueous solution, the Registrant has not indicated that the substance basic aluminium chloride (aluminium hydroxy chloride) would not be stable in the absence of water. Furthermore, it is indicated in open literature that solid polyaluminium chloride products are also available (K.S.Siefert, Polyaluminium chlorides, in Kirk-Othmer Encyclopedia of Chemical Technology, Published Online : 4 DEC 2000, DOI: 10.1002/0471238961.1615122519090506.a01). The information provided in the updated dossier does not allow ECHA to confirm that the water cannot be separated without affecting the stability or the composition of the registered substance.

Therefore, the Registrant is requested to remove water from the constituent section in Section 1.2 of the IUCLID dossier. If the water cannot be removed completely, only the minimum amount necessary for maintaining the substance stability shall be included in the composition of the substance in section 1.2 in the constituents section. However, in this case the Registrant should provide robust scientific justification on why the solvent cannot be removed completely. The justification shall be sufficiently detailed to allow ECHA to verify that all the amount of water reported indeed cannot be removed without affecting the stability of the substance.

If the Registrant considers that the removal of water from the substance will significantly change the composition and nature of the substance, he may report in section 1.2 a composition which excludes water, but where the identities and structures of the aluminium hydroxy chloride constituents are reported as they are present in the aqueous solution and revealed by suitable analytical methods. The concentrations of the constituents can in this case be obtained by back-calculation from the composition of the aqueous solution.

ii) Identification of the constituent "Aluminium (hydroxy) chloride complexes / Polyaluminium Chloride"

For the generic constituent "Aluminium (hydroxy) chloride complexes / Polyaluminium Chloride" the Registrant provided only the generic molecular formula " $Al(OH)_x(Cl)_{(3-x)}$ , with  $x$  ranging from [REDACTED] and typically being [REDACTED]" and generic information about the chemical nature of the complexes, thereby covering all the aluminium hydroxy chloride constituents in the substance with this single group of constituents.

The Registrant should note that in accordance with section 4.2 of the Guidance, the composition shall normally be described up to 100%, and each constituent requires a complete chemical specification, including structural information. For UVCB substances section 4.3 of the Guidance recognizes that they either cannot be fully specified with the IUPAC name of the constituents, as not all the constituents can be identified, or they may be specified with a lack of specificity due to variability of the exact composition. However, also for UVCB substances the chemical composition and the identity of the constituents should still be reported as far as known.

In particular, in accordance with section 4.3 of the Guidance, the following applies:

- All constituents present in the substance with a concentration of  $\geq 10\%$  shall be identified and reported individually;
- All constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually; and
- Other 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 in order to allow ECHA to establish the composition of the substance as manufactured and to use the compositional information as one identifier for the registered substance. This information must also allow ECHA to verify that the composition is consistent with the chemical name reported for the registered substance.

In his comments to the draft decision and in the updated registration dossier, the Registrant described the complexes covered by the generic description as follows: *"This substance is a ionic mixture of different aluminium hydroxide chloride complexes with various degree of polymerisations and various OH/AL molar ratios. The complexes cannot be identified specifically or separated, and their distribution may vary depending on the process variations, even in case of identical aluminium concentrations and molar OH/Al ratios"*.

ECHA takes note of this information. However, although it may not be possible to identify specifically each individual complex in the substance, it is considered that there are powerful analytical techniques available which can e.g. elucidate the environment around Al (such as <sup>27</sup>Al-NMR (Nuclear magnetic resonance) spectroscopy) and more specific information can be obtained on the constituents present in the substance, e.g. on the basis of the oligomerisation degree, speciation (e.g. monomers Al<sup>3+</sup>, Al(OH)<sup>2+</sup>, Al(OH)<sub>2</sub><sup>+</sup>, etc.), and cluster structure type (e.g. Al<sub>13</sub>-Keggin structure).

Therefore, ECHA considers that the indication of a generic group of constituents is not sufficient to allow ECHA to verify the composition, as it would be feasible to obtain more specific information. The Registrant has thus not provided sufficient and appropriate information on the substance composition.

The Registrant is requested to further specify in Section 1.2 the identities of the constituents in the group "Aluminium (hydroxy) chloride complexes / Polyaluminium Chloride", and to divide this generic group into more specific constituents. If specific individual constituents cannot be identified, the Registrant should report groups of constituents on the basis of similar chemical species present in each group. The name and other identifiers for each (group of) constituent(s) shall reflect the nature of the (group) of constituent(s) and specify the stoichiometry, as relevant. If the Registrant considers that it is not possible to report more specific constituents/groups(s) of constituent(s) in section 1.2 he shall include a robust scientific justification for this. In this case, the one generic constituent shall be named in line with the average OH/Al ratio for the specific grade. The more specific information on the nature of the constituents shall be reported in the Description field, and representative structures shall be included in the Structural formula field.

The information provided on the composition shall be sufficient to enable the specific constituents of the substance registered by this legal entity to be identified and shall be consistent with the information included in Section 1.1 on the "name and other identifiers" for the substance. Further technical details on how to report details on the constituents of a substance in IUCLID are available in the "Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH".

In the updated dossier the Registrant has included one composition block named as "Aluminium chloride, basic - Medium OH/Al ratio". However, the Registrant has not indicated whether this is the only grade of the substance that the registration covers. ECHA reminds that if the Registrant covers different grades (i.e. compositions resulting from a specific manufacturing process) 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.

The Registrant should also note that multiple compositions may indicate multiple substances and consequently the requirement for multiple registrations.

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

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.

Initially, the Registrant had not included in Section 1.4 of the IUCLID dossier information that would have enabled the composition of the substance and the stoichiometry of the relevant substance constituents to be verified.

In his comments to the draft decision and the updated dossier the Registrant clarified that, by mistake, some of the information that was initially provided was referring to other substances. In the updated dossier the Registrant indicated clearly which data was relevant for the current registration. The information provided was sufficient to quantify for the tested sample the total amount of aluminium hydroxy chloride in water solution, and the average stoichiometry of the tested sample.

The Registrant described in the Description field of Section 1.2 that the substance consists of a "*mixture of different aluminium hydroxide chloride complexes with various degree of polymerisations and various OH/AL molar ratios*". However, the information included in section 1.4 was not sufficient to confirm this as there was information only on the average stoichiometry of the substance.

Furthermore, as has been explained in section III.A.2 above (Composition of the substance), the Registrant did not provide in the updated dossier sufficiently specific compositional information on the constituents present in the group "Aluminium (hydroxy) chloride complexes / Polyaluminium Chloride". No analytical information was included in section 1.4 which could be considered to give information on these more specific constituents, or as mentioned above, on the nature of the different aluminium hydroxy chloride complexes.

Therefore, the information contained in the dossier regarding the description of analytical methods is not sufficient for the determination of the chemical composition of the substance registered.

In line with Annex VI, 2.3.7, the Registrant shall include information on the methods used to identify and quantify all substance constituents in terms of stoichiometries where relevant. This information shall be sufficient to enable the substance identified in Section 1.1 of the dossier and all constituents reported in Section 1.2 to be verified. Where different compositions of the substance are reported in Section 1.2, sufficient data that will enable each composition to be verified shall be included. The Registrant may use any method or combination of methods to do this (e.g. elemental analysis, gravimetry, quantitative XRD, etc.). Considering the complexity of the aluminium hydroxy chloride complexes it may be appropriate to use also methods which can give more specific information on the Al-containing species, e.g.  $^{27}\text{Al}$ -NMR spectroscopy. The Registrant shall note that a description of each method used shall be included in such detail that the method may be reproduced.

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://echa.europa.eu/regulations/appeals>. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.



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