EUROPEAN CHEMICALS AGENCY

Decision number CCH-D-0000002358-71-04/F Helsinki, 06/09/2012

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

For 1,3,5-tris(oxiran-2-ylmethyl)-1,3,5-triazinane-2,4,6-trione, CAS No 2451-62-9 (EC No 219-514-3), 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 dossier for 1,3,5-tris(oxiran-2-ylmethyl)-1,3,5-triazinane-2,4,6-trione, CAS No 2451-62-9 (EC No 219-514-3) submitted by [redacted] (Registrant), latest submission number [redacted], for the tonnage band of 100 to 1000 tonnes per year.

The compliance check was initiated on 24 April 2012.

On 31 May 2012 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision.

By 2 July 2012 the Registrant did not provide any comments on the draft decision to ECHA.

On 20 July ECHA notified the Competent Authorities of the Member States on its draft decision and invited them pursuant to Article 51(1) of the REACH Regulation to submit proposals to amend the draft decision within 30 days of the receipt of the notification.

Subsequently, Competent Authorities of the Member States did not propose amendments to the draft decision and ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

This compliance check decision does not prevent ECHA to initiate further compliance checks on the present dossier at a later stage.

II. Information required

1) Pursuant to Articles 41(1)(a), 41(3) and 10(a)(ii) as well as Annex VI , section 2 of the REACH Regulation the Registrant shall submit for the registered substance:

   a. Name or other identifiers (Annex VI, 2.1 of the REACH Regulation);

b. Composition of the substance (Annex VI, 2.3 of the REACH Regulation);
c. The description of the analytical methods (Annex VI, 2.3.7 of the REACH Regulation).

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated IUCLID dossier to ECHA by **6 November 2012**.

III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein, submitted by the Registrant for registration of the above mentioned substance for the purpose of registration within the applicable tonnage band of 100 to 1000 tonnes per year in accordance with Articles 6 and 11 of the REACH Regulation, does not comply with the requirements of Articles 10 and 12(d) and with 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.

Missing information related to substance identity:

Pursuant to Article 10(a)(ii) and Annex VI, section 2 of the REACH Regulation, the technical dossier of the registration shall include information on the identity of the substance. Annex VI, section 2 lists information requirements that shall be sufficient to identify the registered substance.

(a) Name or other identifiers (Annex VI, Section 2.1 of the REACH Regulation)

The name and other identifiers are used to identify the substance in an unambiguous manner and are therefore essential parts of substance identification and the corner stone of all the REACH obligations.

ECHA notes that the Registrant identified the registered substance as a mono-constituent substance. In line with the Guidance for identification and naming of substances under REACH (Version: 1.1, November 2011), mono-constituent substances are well-defined substances in which one constituent is present at a concentration ≥ 80% (w/w) (referred to thereinafter as "main constituent"). A mono-constituent substance is named after the name of its main constituent. ECHA observes that the Registrant did not provide appropriate information on the name of the substance, as required under Annex VI Section 2.1 of the REACH Regulation.

More specifically, the Registrant assigned EC and CAS entries and chemical name corresponding to "1,3,5-tris(oxiran-2-ylmethyl)-1,3,5-triazinane-2,4,6-trione" to the registered substance. ECHA observes that such name and identifiers refer to a multi-constituent substance including four main constituents present at concentration [redacted]. More specifically these main constituents correspond to the four stereoisomers:

- 1,3-bis[(2R)-oxiran-2-ylmethyl]-5-[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione, commonly referred to as alpha-isomer
- 1-[(2R)-oxiran-2-ylmethyl]-3,5-bis[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione, commonly referred to as alpha-isomer
- 1,3,5-tris[(2R)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione, commonly referred to as beta-isomer

- 1,3,5-tris[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione, commonly referred to as beta-isomer

The first two stereoisomers are commonly referred to as alpha-isomers, whereas the last two stereoisomers are commonly referred to as beta-isomers. The term alpha-isomer therefore may refer to two different stereoisomers. The same reasoning is valid for the term beta-isomer.

ECHA notes that the Registrant did not provide information on the concentration ratio of all four stereoisomers present in the substance. Instead the Registrant includes the statement: "alpha- and beta-isomers of TGIC exist at a ratio of approx. [redacted]." in section 1.4 of the IUCLID dossier.

According to such statement alpha-isomers are present in the substance in [redacted]% concentration. Beta-isomers, instead, are present in [redacted]% concentration. This means that beta-isomers should be considered as impurities and should not be included in the name of the substance. The substance therefore could include:

- one main constituent in [redacted]% concentration corresponding to one of the two alpha-isomers. In such case the substance may correspond to either the mono-constituent substance
  - 1,3-bis[(2R)-oxiran-2-ylmethyl]-5-[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione

  or the mono-constituent substance
  - 1-[(2R)-oxiran-2-ylmethyl]-3,5-bis[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione

or

- two main constituents corresponding to both alpha-isomers in [redacted]% overall concentration. In such case the substance may correspond to the multi-constituent substance:
  - Reaction mass of 1,3-bis[(2R)-oxiran-2-ylmethyl]-5-[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione and 1-[(2R)-oxiran-2-ylmethyl]-3,5-bis[(2S)-oxiran-2-ylmethyl]-1,3,5-triazinane-2,4,6-trione

It follows that the registration dossier includes contradictory information on the identity of the registered substance.

ECHA points out that, in accordance with the criteria for substance sameness specified in paragraph 5 of the Guidance for identification and naming of substances under REACH, well-defined substances with different main constituents shall be regarded as different substances under REACH. ECHA therefore concludes that the provided EC/CAS entries, chemical name and the composition specified in the dossier refer to different substances.

The Registrant is accordingly requested to provide a chemical name corresponding to the specific substance covered in this registration. The chemical name shall be generated on the basis of the main constituents actually present in the substance.
The Registrant shall also specify any available and appropriate CAS number and CAS name reflecting the identity of the main constituents of the substance. The Registrant shall delete from the registration any information referring to different substances than the substance which is the subject of this registration.

As for the reporting of the information in IUCLID, the chemical name shall be indicated in

the "IUPAC name" field in IUCLID section 1.1. The CAS number and CAS name shall be reported under the "CAS information" header in IUCLID section 1.1. The Registrant is requested not to remove or modify at this stage the EC entry currently assigned to this registration for technical reasons, the registration being linked to that EC entry in REACH-IT.

The Registrant shall ensure that the molecular and structural information specified in IUCLID section 1.1 and the composition indicated in IUCLID section 1.2 are consistent with the chemical name and CAS number and CAS name assigned to the registered substance.

b) Composition of the 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 it is a crucial parameter in its identification.

ECHA notes that the registration does not contain sufficient and appropriate 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, ECHA notes that the Registrant did not provide information on the concentration of each individual stereoisomer present in the composition of the registered substance. The Registrant provided instead cumulated concentration values for alpha-isomers and beta-isomers. It follows that the identity of the main constituents present in the composition of the registered substance cannot be established. ECHA therefore concludes that the composition of the registered substance has not been provided to the required level of detail.
The registrant is accordingly requested to provide information on the concentration values of the stereoisomers present in the substance which is the subject of this registration.

In addition, ECHA notes that the information provided on the composition of the substance is inconsistent with the results of the analytical data provided. More specifically the concentration ranges specified for the constituents present in the substance, including impurities, are not aligned with the concentration values indicated in the analytical report, as a result of the LC-MS and HPLC analyses.
ECHA therefore cannot conclude which concentration ranges correspond to the constituents and impurities present in the substance.
The Registrant is therefore requested to revise the information given in the composition section of the IUCLID dossier.

In line with paragraph 4.3 of the Guidance for identification and naming of substances under REACH and CLP, the following applies to all well-defined substances, including the registered substance:

- All main constituents shall be identified and reported individually; and
- All the impurities present at ≥ 1 % shall be identified and reported individually; and
- All the impurities relevant for the classification and/or PBT assessment shall be identified and reported individually.

For each constituent, including the main constituents and any impurity, the typical, minimum and maximum concentration level shall be specified.

The Registrant is accordingly requested to complete the above information on the composition of the registered substance provided in the registration dossier, for ECHA to

have a precise chemical representation of what the specific well-defined substance, which is the subject of this registration, consists of.

Regarding how to report the composition in IUCLID, the following applies: The Registrant shall report individually each main constituent and 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 IUCLID section 1.2.

The Registrant shall ensure that the compositional information is verifiable and therefore supported by a description of the analytical methods used for the identification and quantification of each constituent required to be reported, as specified under Annex VI section 2.3.7 of the REACH Regulation.

c) The description of the analytical methods (Annex VI, 2.3.7 of the REACH Regulation)

ECHA notes that the Registrant provided a HPLC/UV chromatogram as a quantitative analysis of the registered substance. However such information is not sufficient to establish the concentration ratio of the isomers present in the substance. ECHA therefore concludes that the provided chromatographic analysis cannot be used as such to draw any conclusion on the composition of the registered substance and on the quantification of all its constituents.

The Registrant is accordingly requested to provide a description of the analytical methods used for the identification and quantification of all the isomers included in the substance. The Registrant should demonstrate how the results of the chromatographic analysis have been translated into concentrations of the constituents present in the 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.

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/appeals/app_procedure_en.asp. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

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Jukka MALM
Director of Regulatory Affairs