EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000003604-77-03/F Helsinki, 1 October 2013

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

For 1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters, CAS No 68515-40-2 (EC No 271-082-5), 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 1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters, CAS No 68515-40-2 (EC No 271-082-5) submitted by [redacted] (Registrant). The scope of this compliance check is limited to the standard information requirements of Annex VI, 2.1., 2.3., 2.3.5., 2.3.6. and 2.3.7. 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 20 June 2013, 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.

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 20 April 2012.

On 19 April 2013 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 20 May 2013 the Registrant did not provide any comments on the draft decision to ECHA.

On 20 June 2013 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 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.

II. Information required

Pursuant to Articles 41(1)(a), 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 or other identifier of the substance (Annex VI, 2.1.), as specified under section III.a) below;
b) The composition (Annex VI, 2.3.), as specified under section III.b) below;
c) Spectral data (Annex VI, 2.3.5.) , as specified under section III.c) below;
d) Chromatogram (Annex VI, 2.3.6.);
e) The description of the analytical methods or the appropriate bibliographical references for the identification of the substance (Annex VI, 2.3.7.), as specified under section III.e) 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 January 2013.**

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.

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.

a) Name or other identifier of the substance (Annex VI, 2.1.)

ECHA observes that the Registrant provided EC and CAS identifiers that are specific for the substance of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB) "1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters". The substance described by such name includes a multitude of isomeric constituents bearing C7, C8 and C9 branched and linear alkyl chains and is therefore considered as a UVCB substance. ECHA however notes that the Registrant identified the registered substance as a mono-constituent substance in IUCLID Section 1.1.Therefore the information provided is inconsistent with the information provided on the EC and CAS identifiers.

Furthermore, ECHA notes that the structural formula provided for the registered substance specifies the presence of C7-C9 linear alkyl chains, and specifies that only C9 alkyl chains are branched. This information is inconsistent with the EC and CAS identifiers provided which refer to a substance including also C7 and C8 branched alkyl chains. Therefore the information provided is also inconsistent with respect to which groups of constituents present in the substance show branched alkyl chains.

As the information provided by the Registrant pursuant to Annex VI, Section 2.1. is inconsistent, the Registrant is required to revise the information provided and ensure its consistency.

If the substance is indeed a UVCB substance, the registrant shall keep in mind the specific requirements for naming of the registered substance.

The registrant shall note that the naming of UVCB substances shall consist of two parts: the chemical name and a more detailed description of the manufacturing process as described in chapter 4.3 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.2, March 2012) – referred to as "the Guidance" hereinafter. ECHA notes that the Registrant did not provide appropriate information for the naming of the registered substance, as required under Annex VI Section 2.1 of the REACH Regulation.

The Registrant shall provide an appropriate chemical name which needs to be filled in the "IUPAC name" field, as indicated in chapter 8.2.4 of the Guidance for the registered substance. Such inclusion of the IUPAC name in the proper field is necessary for its correct identification. In addition ECHA notes that the description of the manufacturing process provided in IUCLID section 3.1 is not sufficiently detailed to identify the registered substance. More specifically, the Registrant identified one of the starting materials used for the manufacturing of the registered substance as "alcohol". The identity of the exact starting material has not been provided. Compositional information of that starting material (in terms of identity and upper and lower concentration levels of the linear and branched alcohols presenting the same carbon number) is necessary for the identification of the registered substance. Furthermore, no information was provided on the ratio of the starting materials.
For this purpose, the Registrant shall provide a chemical name that is representative of the registered substance. The registrant shall, in addition, provide the missing information on the identity and composition of the starting materials used, on the ratio of the starting materials and on any manufacturing process parameters which determine the composition of the registered substance and therefore its identity.

The registrant shall ensure that the information given on the name of the registered substance is consistent with the structural formula and the identifiers provided.

If the registered substance does not correspond specifically to the substance described by the CAS entry "1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters", CAS entry 68515-40-2 can be reported under the "Related CAS information" header in IUCLID section 1.1. In such case, 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 is requested to include the following in the "Remarks field" of the reference substance: "The EC entry currently assigned does not specifically correspond to the registered substance. This identifier cannot be modified in the present registration at this stage for technical reasons".

Regarding how to report the chemical name and description of the manufacturing process of the UVCB substance, the information shall be included in the IUPAC name field and the Description field in IUCLID section 1.1, respectively.

b) The 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 information that is sufficient for

establishing the composition of the registered substance, as required under Annex VI, Section 2.3. of the REACH Regulation. More specifically, ECHA notes that the Registrant has provided information on the typical concentration of a generic group of constituents corresponding to "1,2-Benzenedicarboxylic acid, benzyl C7-9-branched and linear alkyl esters". ECHA points out that the Registrant did not specify any information on the specific groups of constituents present in the substance. Typical concentration and concentration ranges of the specific constituents/groups of constituents bearing linear and branched alkyl chains and presenting the same carbon number have not been given in the registration dossier. It follows that the composition of the registered substance cannot be established and is therefore considered missing from the dossier.

Furthermore the result of the gas chromatography-mass spectroscopy GC/MS included in the analytical report "GCMS S261A" shows the presence of several constituents that have not been included in the composition information in section 1.2 of the IUCLID dossier. According to the Guidance chapter 4.3, the Registrant should note that, for UVCB substances, 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 unknown 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 substances such as the registered substance, a distinction of the unknown constituents according to the carbon number and backbone type (linear, branched) is necessary for this purpose as a baseline. The ratio of the linear and brached constituents shall be provided for each individual carbon number.

For each constituent or group of constituents, the typical, minimum and maximum concentration levels 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 substance consists of.

Regarding how to report the composition in IUCLID, the following applies: The Registrant shall indicate 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 reported in the appropriate fields in IUCLID. For the other constituents to 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 reported in the appropriate fields in IUCLID.

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: 1.0, June 2010).

The Registrant shall ensure that the information provided on the composition is consistent with the identity of the Registered UVCB substance and is confirmed by the analytical data included in section 1.4 of the IUCLID dossier.

c) Spectral data (Annex VI, 2.3.5.)

ECHA observes that the Registrant provided an infra-red (IR) spectrum including the remark:" Reference spectra from S261A were copied from the Antwerp Library. Those spectra were taken with Smart orbit on the Nicolet 380." It is not clear if the spectrum given was obtained from the substance as manufactured or if it is a copy of a spectrum present in the database of a library.

In addition ECHA notes that the registration does not contain any appropriate nuclear magnetic resonance (NMR) or mass spectra required according to Annex VI Section 2.3.5. of the REACH Regulation to support the identity of the registered substance.

ECHA notes that the Registrant attached to the dossier a report from a gas chromatography-mass spectroscopy (GCMS) analysis of the registered substance. The report includes a copy of a chromatogram and a number of mass spectra. However, ECHA cannot relate the provided mass spectra to the recorded chromatogram. These spectra do not appear to be generated from the GCMS analysis of the registered substance but to originate instead from mass spectral libraries, as for instance in the case of the spectrum assigned to phthalic anhydride which refers to "mainlib". In addition, the mass spectra for all the constituents detected, including the main constituents eluting at ca. 22 min have not been included. ECHA therefore cannot use the mass spectral data included in the registration to verify the identity of the constituents present in the composition of the registered substance.

The Registrant shall ensure that IR spectrum attached to the IUCLID dossier is obtained from the substance as manufactured.
Furthermore the Registrant is requested to submit appropriate NMR spectra (such as a ^{1}H and ^{13}C NMR spectra, including also, where relevant, the peak integrals) to support the identity of the constituents present in the composition of the registered substance. As an alternative or in complement to NMR spectra, mass spectra of the registered substance shall be provided. This information shall be sufficient for the identification of the substance including its constituents.

As for the reporting of the spectral data in the registration dossier, the information shall be included in IUCLID section 1.4.

The Registrant shall ensure that the description of the analytical methods used for the recording of the spectra is specified in the dossier, in line with the requirements under Annex VI section 2.3.7.

d) Chromatogram (Annex VI, 2.3.6.)

ECHA notes that a copy of a gas-chromatogram (GC) has been attached to the dossier. However, ECHA observes that the Registrant did not provide any report from this chromatographic analysis. In particular, a peak table with the associated retention times and peak area has not been included in the IUCLID dossier. ECHA points out that this information is required since it constitutes a numerical representation of the chromatogram.

The Registrant is accordingly requested to provide the report from the chromatographic analysis of the registered substance.

As for the reporting in the registration dossier, the information shall be included in IUCLID section 1.4.

e) Description of the analytical methods (Annex VI, section 2.3.7.)

ECHA observes that the Registrant did not provide any appropriate description of the analytical methods used for the identification and quantification of the constituents required to be reported in the composition of the registered substance, as requested according to Annex VI section 2.3.7.

More specifically ECHA notes that the Registrant provided results from an analytical method based on GC chromatography. However, the protocol followed to record the chromatogram (including details of the sample preparation, the column specifications, identity of the carrier gas used, temperature applied, identity of the internal standards) has not been included in the analytical report. It follows that the results of these analyses cannot be reproduced. In addition, the description of the analytical methods used for the identification and quantification of each group of constituents expected to be present in the composition of the registered substance and quoted under point III.(a) of this decision is missing from the dossier.

The Registrant is accordingly requested to provide a description of the analytical methods used for the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance, according to the carbon number and backbone type (linear, branched). 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.

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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