EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004494-71-03/F Helsinki, 20 August 2014

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

For butan-2-ol, CAS No 78-92-2 (EC No 201-158-5), 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 butan-2-ol, CAS No 78-92-2 (EC No 201-158-5), submitted by [redacted] (Registrant). The scope of this compliance check is limited to the standard information requirements of Section 2 of Annex VI, while the compliance check concerning the information requirements laid down in Annex I and Annexes VII to X was done on the lead registrant dossier of this joint submission.

This decision is based on the registration as submitted with submission number [redacted], for the tonnage band of 1000 tonnes or more tonnes per year. This decision does not take into account any updates submitted after 6 March 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.

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 8 October 2013.

On 18 November 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.

On 17 December 2013 ECHA received comments from the Registrant agreeing on the draft decision.

The ECHA Secretariat considered the Registrant's comments and decided not to amend the draft decision.

On 6 March 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)(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:

1. Information on optical activity and typical ratio of (stereo) isomers (Annex VI, 2.2.2)
2. Spectral data (nuclear magnetic resonance) (Annex VI, 2.3.5)

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 **27 November 2014**.

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.

1. Information on optical activity and typical ratio of (stereo) isomers (Annex VI, 2.2.2)

"Information on optical activity and typical ratio of (stereo) isomers" is an information requirement as laid down in Annex VI, Section 2.2.2. of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

The Registrant has stated the following under optical activity in section 1.4 of the IUCLID dossier: *"See below"*, but no further explanation or attachment was included. In addition, in the manufacturing process provided in section 3.1 of the IUCLID dossier it is stated that *"Produced by hydration of n-butene"*.

ECHA notes that the main constituent reported in the composition for the registered substance, in section 1.2 of the IUCLID dossier, contains one stereocentre. Thus, according to Annex VI, Section 2.2.2. of the REACH Regulation, information on the optical activity and the typical ratio of stereoisomers should have been reported. This information has not been provided by the Registrant and consequently there is an information gap.

Regarding how to report the composition of the registered substance in IUCLID, the Registrant shall specify the ratio of stereoisomers in the Remarks field of the repeatable block created for each group of constituents in IUCLID section 1.2. Alternatively, the Registrant can report separately each individual stereoisomer, including information on their typical, minimum and maximum concentration in IUCLID section 1.2.

The Registrant shall ensure that the information on the stereochemistry is verifiable and therefore supported by a description of the analytical methods used for the quantification, as required under Annex VI section 2.3.7. of the REACH Regulation.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: report the ratio of the different isomers present in the composition of the registered substance as specifically explained above. The Registrant shall ensure that the information is consistent throughout the dossier.

2. Spectral data (nuclear magnetic resonance) (Annex VI, 2.3.5)

"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) data for the identification of the main constituent of the registered substance, which is required according to Annex VI, Section 2.3.5. of the REACH Regulation to support the identity of the registered substance.

ECHA points out that the identity of the substance cannot be confirmed based exclusively on the ultra-violet (UV) and infrared (IR) spectra. NMR spectroscopic analyses such as a 1H-NMR or a 13C-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, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: nuclear magnetic resonance data as specifically explained above. Alternatively, a mass spectrum including the corresponding interpretation of the fragmentation scheme can be provided. The Registrant shall ensure that the information is consistent throughout the dossier.

As for the reporting of the spectral data in the registration dossier, the information should be included 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/regulations/appeals. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

[redacted]
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Director of Evaluation