EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004536-71-03/F Helsinki, 11 August 2014

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

For xylene, CAS No 1330-20-7 (EC No 215-535-7), 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 xylene, CAS No 1330-20-7 (EC No 215-535-7), 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 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 24 September 2013.

On 18 December 2013 ECHA sent the draft decision to the Registrant and invited him to provide comments within 45 days of the receipt of the draft decision.

On 3 February 2014 ECHA received comments from the Registrant on the draft decision.

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

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. Name or other identifier of the substance (Annex VI, Section 2.1.), as specified in Section III.1. below;
2. Composition of the substance (Annex VI, Section 2.3.), as specified in Section III.2. below;
3. Spectral data (Annex VI, Section 2.3.5.), as specified in Section III.3. below;
4. Description of the analytical methods or the appropriate bibliographical references for the identification of the substance (Annex VI, Section 2.3.7.) as specified in Section III.4. 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 **18 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. Name or other identifier of the substance (Annex VI, Section 2.1.)

According to Annex VI, Section 2.1 of the REACH Regulation, name or other identifier of each substance shall be provided. This includes the name in the IUPAC nomenclature or other international chemical name(s) (Annex VI, Section 2.1.1); as well as CAS name and CAS number (if available) (Annex VI, Section 2.1.4).

In accordance with the Guidance for identification and naming of substances under REACH and CLP (Version: 1.2, March 2012)[1] - referred to as "the Guidance" thereinafter, a substance is defined as a Unknown or Variable composition, Complex reaction products or Biological materials (UVCB) when the number of constituents is relatively large and/or the composition is to a significant part unknown and/or the variability of composition is relatively large or poorly predictable. The Guidance also defines multi-constituent substances as well-defined substances in which more than one constituent is present at a concentration >10% (w/w) and <80% (w/w) (referred to thereinafter as "main

[1] http://echa.europa.eu/documents/10162/13643/substance_id_en.pdf

constituent"). A multi-constituent substance is named as the reaction mass of the main constituents.

ECHA notes that the Registrant has identified the registered substance as a UVCB. However, analytical data included in the registration dossier and the sum of the typical concentration values specified for the identified constituents clearly indicate that the registered substance has a well-known composition. As a consequence, in accordance with the Guidance, the registered substance should rather be regarded as a multi-constituent substance.

Moreover, ECHA notes that the name provided (xylene) and the numerical identifiers used for defining the registered substance (EC number 215-535-7 and CAS number 1330-20-7) refer to a substance containing all the possible isomers of xylene (ortho-, meta- and para-xylene). However, the IUPAC name and identifiers used to identify the substance do not reflect the substance composition. The composition of the substance provided in section 1.2 of the IUCLID dossier shows that ethylbenzene is present at a typical concentration >10% (w/w). As a consequence, ECHA considers that the IUPAC name provided by the Registrant is not representative of the composition of the registered substance, because the presence of the main constituent ethylbenzene is not reflected in the name of the substance.

Therefore, ECHA concludes that the provided chemical name and EC/CAS entries do not reflect the substance composition as substantiated by the provided analytical data.

The Registrant is accordingly requested to provide a chemical name corresponding to the specific multi-constituent substance covered in this registration. The chemical name shall follow the generic format "Reaction mass of [names of the main constituents]". All main constituents present in the registered substance shall be reflected in the name of the registered 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 multi-constituent 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 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".

Furthermore, the Registrant shall ensure that the molecular and structural information specified in IUCLID section 1.1 (smiles notation, InChI code and structural formula) are consistent with the chemical name and CAS number and CAS name assigned to the registered substance.

Finally, 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 and CLP, multi-constituents substances with different main constituents shall be regarded as different substances and subject to different registrations under the REACH Regulation.

2. Composition of the substance (Annex VI, Section 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 exact 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 has not specified any information on the minimum and maximum concentration values of the different constituents reported in IUCLID Section 1.2. Therefore, ECHA cannot conclude on the composition of the registered substance and the variation of these constituents.

The Registrant is accordingly requested to submit information on the constituents of the registered substance and information on the variation of these constituents in the composition of the substance. This information is essential to enable ECHA to have a precise chemical representation of what the substance consists of. The Registrant shall ensure that the information provided on the composition of the substance is consistent with the identity of the registered substance.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: the Registrant shall report the composition 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. Further technical details on how to report the composition of well-defined substances in IUCLID are available in paragraphs 2.2.1. of the Data Submission Manual 18 on the ECHA website.[2]

3. Spectral data (Annex VI Section 2.3.5.)

ECHA observes that the registration does not contain the Ultra-Violet (UV) and Nuclear Magnetic Resonance (NMR) or Mass Spectrum (MS) spectral data 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 spectral data Ultra-Violet (UV), Infra-Red (IR) and Nuclear Magnetic Resonance (NMR) or Mass Spectrum (MS) are a formal information requirement under Annex VI section 2.3.5. of REACH.

ECHA regards this required information scientifically relevant for the registered substance for the following reasons:
- The substance absorbs in the UV range due to the presence of chromophores in the composition. A UV spectrum representing the absorption of these constituents in the UV range can therefore be recorded;
- 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 reflects the relative abundance of individual atoms.

[2] http://echa.europa.eu/documents/10162/13653/substance_id_report_iuclid_en.pdf

The Registrant is therefore requested to submit a UV spectrum and an NMR spectrum, such as a 1H-NMR or a 13C-NMR. As an alternative to an NMR spectrum, mass spectrum (MS) generated as part of mass spectroscopic analysis for the elucidation of the structure of the constituents in the substance can be provided. This MS should include an explanation of the substance specific mass pattern observed in the spectrum.

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

The Registrant shall ensure that the description of the analytical methods used for the recording of the UV and NMR or MS spectra are specified in the dossier, in line with the requirements under Annex VI section 2.3.7.

4. Description of the analytical methods for the identification of the substance (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. of the REACH Regulation.

ECHA notes that the gas chromatogram reported in Section 1.4 of the IUCLID dossier indicates the presence of several individual peaks. However the Registrant did not provide any description of the method used to translate the analytical results into the composition required to be reported in Section 1.2 of the IUCLID dossier.

In addition, the reported gas chromatogram shows a main peak around 19 min that is not accounted for by the Registrant in the table listing the individual constituents of the registered substance and in Section 1.2 of the IUCLID dossier.

ECHA therefore concludes that an appropriate description of the analytical methods used for the identification of the registered substance 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 required to be reported in the composition of the registered substance. This method should report a quantitative analysis allowing the quantification of all the individual xylene isomers and any other relevant constituent. The composition reported in section 1.2 should then be consistent with the analytical information provided in section 1.4. Finally, 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 above data in the registration dossier, the information should be attached in IUCLID section 1.4.

During the commenting phase the Registrant proposed to "submit before the end of 2014 a spontaneous update addressing the issues raised within the draft decision, specifically on substance identification". The Registrant substantiates the proposal stating that "this time is required as careful discussion with all the registrants will be required as it may have unintended consequences to the supply chain which will need to be resolved."

ECHA acknowledges the Registrant's commitment to update the substance identity information as required by the present decision. However, ECHA considers that the deadline provided (3 months from the date of the decision) is sufficient to consider consequences in the supply chain as well as to update the substance identity information according to the requests formulated in the present decision. In fact, ECHA considers the information requested as administrative, hence the need for a longer deadline is not justified.

Therefore, the requests and deadline set in the decision are maintained and the Section II of the decision is not amended based on the comments provided by the Registrant.

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.

Leena Ylä-Mononen
Director of Evaluation