Helsinki, 23 September 2016

Addressee [redacted]

Decision number: CCH-D-2114343415-54-01/F
Substance name: tert-butyl-4-methoxyphenol
EC number: 246-563-8
CAS number: 25013-16-5
Registration number: [redacted]
Submission number: [redacted]
Submission date: 09.09.2015
Registered tonnage band: 100-1000T

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (the 'REACH Regulation'), ECHA requests you to submit information on

1. **Name or other identifier of the substance (Annex VI, Section 2.1.);**
2. **Composition (Annex VI, Section 2.3.) of the registered substance;**
3. **Spectral data (Annex VI, Section 2.3.5) on the registered substance;**
4. **High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6) of the registered substance;**

You are required to submit the requested information in an updated registration dossier by **3 January 2017**. You shall also update the chemical safety report, where relevant.

The reasons of this decision are set out in Appendix 1. The procedural history is described in Appendix 2. Advice and further observations are provided in Appendix 3.

The scope of this compliance check decision is limited to the standard information requirement(s) of Annex VI, Section 2 of the REACH Regulation.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, shall be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under http://echa.europa.eu/regulations/appeals.

Authorised[1] by Ofelia Bercaru, Head of Unit, Evaluation E3

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

ECHA
EUROPEAN CHEMICALS AGENCY

Appendix 1: Reasons

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.)

The name and other identifiers are used to identify the substance in an unambiguous manner and are therefore fundamental for substance identification. Adequate information needs to be present in the registration dossier to meet this information requirement.

Annex VI section 2 of the REACH Regulation requires that each registration dossier contains sufficient information to enable the registered substance to be identified.

According to chapter 4.2.2 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.3, February 2014) – referred to as "the Guidance" thereinafter, a mono-constituent substance is a substance in which one constituent is present at a concentration of at least 80% (w/w) and which contains up to 20% (w/w) of impurities. In contrary, a multi-constituent substance is a substance defined by its composition, for which more than one main constituent is present at a concentration ≥ 10% (w/w) and < 80% (w/w).

You assigned EC number 246-563-8, EC name "tert-butyl-4-methoxyphenol" and CAS number 25013-16-5 corresponding to "tert-butyl-4-methoxyphenol" in section 1.1 of the registration dossier. ECHA observes that the chemical name "[redacted]" refers to a multi-constituent substance consisting of [redacted] and [redacted] as main constituents.

However, the IUPAC name "[redacted]", structural formula, SMILES notation and InChI code provided in section 1.1 refer to a mono-constituent substance [redacted]

Furthermore, ECHA notes that you have indicated that the type of substance is "mono-constituent substance" in the Composition-field in section 1.1.

The EC number, EC name and CAS number are not consistent with the IUPAC name, structural formula, SMILES notation and InChI code reported in section 1.1.

Furthermore, the type of substance is not consistent with the EC number, EC name and CAS number reported in section 1.1.

Therefore, you are requested to revise the identifiers reported in section 1.1 and to ensure that the identifiers are representative of the specific substance which is the subject of this registration. The identifiers reported in section 1.1 must be consistent with the composition reported in section 1.2 of the IUCLID dossier and the analytical data attached in section 1.4 of the IUCLID dossier.

Regarding how to report the identifiers of the substance, the information shall be included in the reference substance assigned in IUCLID section 1.1.

You shall ensure to select the "type of substance" corresponding to the substance subject to this registration from the appropriate dropdown list in section 1.1 of the IUCLID dossier. You shall ensure that the correct identifiers are used throughout the registration whenever reference to the specific substance which is the subject of this registration is made. If you select "multi-constituent substance" as type of substance, you shall, for technical reasons, do the following in section 1.2 of the IUCLID dossier:

- Include the following statement in the "Brief description" field of the composition currently reported in section 1.2 of the IUCLID dossier: "This composition block does not describe the registered multi-constituent substance and is reported only for technical reasons"; and

- Create a second composition block describing the composition of the multi-constituent substance. For this second composition, ECHA reminds that all the main constituents shall be listed under the "Constituents" header.

If the current identifiers are not appropriate to describe the registered substance, you should not remove or modify at this stage this EC entry for technical reasons, the registration being linked to that EC entry in REACH-IT. To ensure unambiguous identification of the registered substance, you should however indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC number 246-563-8 currently assigned does not specifically correspond to the registered substance. This identifier cannot be modified or deleted at this stage in the present registration update for technical reasons". You should also specify, in the same "Remarks" field, any available and appropriate EC number for the substance. Any available CAS entry for the registered substance should be reported under the "CAS information" header of the reference substance in IUCLID section 1.1.

You should note that ECHA has established a process, subject to certain conditions, enabling registrants to adapt the EC identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned.

Pending the resolution of the non-compliances addressed in the present decision, any possible adaptation of the identifier can only become effective once ECHA is in a position to establish unambiguously the identity of the substance intended to be covered by you with this registration. Should the information submitted by you as a result of the present decision enable ECHA to identify the substance unambiguously and result in a need to modify the identifier of the substance, the process of adapting the identifier will be considered relevant. In that case, ECHA will inform you in due time as to when and how the identifier adaptation process shall be initiated.

In any case, you should note that the application of the process of adapting the identifier does not affect your obligation to fulfil the requirements specified in this decision.

2. Composition of the substance (Annex VI, Section 2.3.)

Annex VI, section 2.3. of the REACH Regulation requires that each registration dossier contains sufficient information for establishing the composition of the registered substance and therefore its identity.

In that respect, according to chapter 4.2 of the Guidance, you shall note that, for well-defined substances, the following applies:

- Each main constituent (i.e. the constituent present at ≥80% for mono-constituent substance or each constituent present at ≥10% and 80% for multi-constituent substance) shall be identified and reported individually; and

- Each impurity present at ≥1% or relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually.

- For each constituent, the typical, minimum and maximum concentration levels shall be specified regardless of the substance type.

ECHA notes that you have only reported one reference substance with EC number [redacted], EC name "[redacted]", CAS number [redacted] and IUPAC name "[redacted]" in section 1.2. The presence of other constituents or impurities was not indicated in the reported composition.

You assigned EC number [redacted], EC name "[redacted]" and CAS number [redacted] corresponding to "[redacted]" for the reference substance reported in section 1.2 of the registration dossier. ECHA observes that the chemical name "[redacted]" refers to a group of constituents consisting of [redacted] and [redacted].

However, the IUPAC name "[redacted]", structural formula, SMILES notation and InChI code provided for the reference substance reported in section 1.2 refer to [redacted].

The EC number, EC name and CAS number provided for the reference substance reported in section 1.2 are not consistent with the IUPAC name, structural formula, SMILES notation and InChI code.

Furthermore, ECHA concludes that the compositional information has either (1) not been provided to the required level of detail or (2) is insufficiently reported.

You are accordingly requested to correct the composition reported in section 1.2 and to ensure that the identifiers provided for the reference substance(s) reported in section 1.2 are consistent.

For this purpose, each main constituent (i.e. the constituent present at ≥80% for mono-constituent substance or each constituent present at ≥10% and 80% for multi-constituent substance) must be identified and reported individually in section 1.2.

- If the substance consists of both [redacted] and [redacted] as main constituents, these constituents need to be reported separately in section 1.2, and the typical, minimum and maximum concentration values need to be specified for each constituent.

- If the substance consists of only one main constituent, the main constituent needs to be reported separately in section 1.2, and the typical, minimum and maximum concentration values need to be specified for the constituent.

The reported composition must be consistent with the identifiers reported in section 1.1 of the IUCLID dossier and verifiable by the analytical information provided in section 1.4 of the IUCLID dossier.

The composition shall be reported 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, should 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 the Data Submission Manual – Part 18: How to report the substance identity in IUCLID 5 for registration under REACH (version: 2.0, July 2012) on the ECHA website.

You shall ensure that the composition is verifiable and therefore supported by a description of the analytical methods for the identification and quantification of the constituents required to be reported, as required under Annex VI Section 2.3.7. of the REACH Regulation. 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.

3. Spectral data (Annex VI, Section 2.3.5.)

Spectral data are a formal information requirement of Annex VI Section 2.3.5.

You assigned EC number 246-563-8, EC name "tert-butyl-4-methoxyphenol" and CAS number 25013-16-5 corresponding to "tert-butyl-4-methoxyphenol" in section 1.1 of the registration dossier. ECHA observes that the chemical name "[redacted]" refers to a multi-constituent substance consisting of [redacted] and [redacted] as main constituents.

The IUPAC name "[redacted]", structural formula, SMILES notation and InChI code provided in section 1.1 refer to a mono-constituent substance [redacted].

The 1H-NMR spectrum attached in section 1.4 of the IUCLID dossier does not confirm the identity of the registered substance. More specifically the spectrum does not show the expected signal corresponding to the methoxy group bound to the aromatic ring.

You are therefore requested to submit an NMR spectrum, such as a 1H-NMR or a 13C-NMR, that confirms the identity of the registered substance. A full interpretation of the spectra, including peak assignment, should be provided in order to confirm the structure of the substance. As an alternative to an NMR spectrum, mass spectra (MS) generated as part of mass spectroscopic analysis for the elucidation of the structure of the constituent(s) in the substance can be provided.

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

4. High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.)

"High-pressure liquid chromatogram, gas chromatogram" is an information requirement as laid down in Annex VI, Section 2.3.6. of the REACH Regulation. Adequate information needs to be present in the registration dossier to meet this information requirement.

You have provided a high-pressure liquid chromatogram in section 1.4 of the IUCLID. However, the chromatogram shows only one (group of) peak(s) with retention time of approximately 2.5 minutes. The form of the (group of) peak(s) indicates that this (group of) peak(s) consists of up to three peaks that have not been resolved with the chromatographic method.

Therefore, ECHA concludes that the applied chromatographic method is not sufficient for the quantification of the registered substance and the quantification of the constituents and impurities required to be reported in the IUCLID dossier.

ECHA notes that you assigned EC number 246-563-8, EC name "tert-butyl-4-methoxyphenol" and CAS number 25013-16-5 corresponding to "tert-butyl-4-methoxyphenol" in section 1.1 of the registration dossier. ECHA observes that the chemical name "[redacted]" refers to a multi-constituent substance consisting of [redacted] and [redacted] as main constituents. If the substance consists of both [redacted] and [redacted] as main constituents, the analytical information provided in section 1.4 must be sufficient to quantify these constituents separately.

You are accordingly requested to derive the composition on the basis of the most appropriate method that provides sufficient peak separation. For this purpose, you should submit an appropriate chromatographic analysis including the chromatogram and a peak table containing the retention times, peak areas and peak area % of the constituents. If other analytical methods are more suitable for quantification of the constituents required to be reported in section 1.2, such methods may also be used.

You should also provide a description of the analytical methods used for the identification and quantification of the constituents and impurities required to be reported in the composition of the registered 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.

When reporting the composition of registered substance you shall take into account the uncertainty of the results obtained. You shall ensure that the concentration levels of the constituents and impurities present in the substance are not underestimated.

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

Appendix 2: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of your registration after the date when the draft decision was notified to you under Article 50(1) of the REACH Regulation.

The compliance check was initiated on 13 April 2016.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments.

ECHA did not receive any comments by the end of the commenting period.

ECHA notified the draft decision to the competent authorities of the Member States for proposal(s) for amendment.

As no amendments were proposed, ECHA took the decision according to Article 51(3) of the REACH Regulation.

Appendix 3: Further information, observations and technical guidance

1. The substance subject to the present decision is provisionally listed in the Community rolling action plan (CoRAP) for start of substance evaluation in 2015.

2. This compliance check decision does not prevent ECHA from initiating further compliance checks on the present registration at a later stage.

3. Failure to comply with the request(s) in this decision, or to fulfil otherwise the information requirement(s) with a valid and documented adaptation, will result in a notification to the enforcement authorities of your Member State.