EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004652-75-03/F Helsinki, 30 May 2014

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

**For tris(methylphenyl) phosphate, CAS No 1330-78-5 (EC No 215-548-8), 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 tris(methylphenyl) phosphate, CAS No 1330-78-5 (EC No 215-548-8), 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 100 to 1000 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.

The substance subject to the present decision is provisionally listed in the Community rolling action plan (CoRAP) for start of substance evaluation in 2014.

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 14 November 2013.

On 17 December 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 30 January 2013 ECHA received comments from the Registrant agreeing to ECHA's draft decision

The ECHA Secretariat considered the Registrant's comments but Section II of the draft decision was not amended.

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), 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, 2.1.);
2. Percentage of (significant) main impurities (Annex VI, 2.3.3.);
3. High-pressure liquid chromatogram or gas chromatogram (Annex VI, 2.3.6.);
4. Description of the analytical methods or appropriate bibliographical references for the identification of the substance (Annex VI, 2.3.7.).

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 **08 September 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, 2.1.)

The Registrant identified the registered substance as a multi-constituent substance. In line with chapter 4.2.2 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.2, March 2012) - referred to as "the Guidance" thereinafter, multi-constituent substances are 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 constituent"). A multi-constituent substance is named as the reaction mass of the main constituents. 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 the EC and CAS entries for "tricresyl phosphate" to the registered substance and provided a structural formula corresponding to this substance. Tricresyl phosphate corresponds under REACH to a substance composed of all

possible isomers of tricresyl phosphate as main constituents and does not correspond to a substance that includes a limited number of isomers of tris(methylphenyl) phosphate. However, ECHA notes that the IUPAC name, InChI and SMILES notations indicated in section 1.1 of the IUCLID dossier refer to a specific isomeric form of tricresyl phosphate namely tris(**4**-methylphenyl) phosphate.

Furthermore, the compositional information provided in section 1.2 and the analytical data attached in section 1.4 of the IUCLID dossier do neither confirm the predominance of a specific isomer nor the presence of all possible isomers of the tricresyl phosphate. More specifically, the compositional information describes a multi-constituent substance with three different isomers of tricresyl phosphate as main constituents namely

- Tris(**3**-methylphenyl) phosphate,
- **4**-Methylphenyl **di-3**-methylphenyl Phosphate and
- **3**-Methylphenyl **di-4**-methylphenyl Phosphate.

The isomeric form (tris(**4**-methylphenyl)phosphate is instead reported as an impurity.

In accordance with section 5 ("Criteria for checking if substances are the same") of the Guidance, a substance including all possible isomers is not regarded equal to a substance with only a subset of the possible isomers (c.f. the example of Difluorotoluenes provided in the Guidance). Based on the compositional information provided, the registered substance consists of a subset of all possible isomeric constituents of tris(3-methylphenyl)phosphate. In line with the Guidance such subset cannot be regarded as equal to the substance identified by EC 215-548-8. Multi-constituent substances with different main constituents shall be regarded as different substances under REACH. As a consequence the EC (and CAS) entry currently specified in the registration dossier is not appropriately identifying the substance that is actually manufactured.

Accordingly, the Registrant is requested to clarify the identity of the substance by providing consistent name and other identifiers of the substance. The chemical name shall reflect the presence of the specific isomeric forms of tricresyl phosphate included in the registered substance as main constituents. The chemical name shall follow the generic format "Reaction mass of [names of the main constituents]". The chemical (IUPAC) name and other identifiers shall be included in the corresponding fields of IUCLID section 1.1. If none of the existing CAS entries can precisely describe the registered substance, the CAS field shall be left empty and the CAS number 1330-78-5 shall be moved to the "Related CAS information" field, if appropriate.

Concerning the modification of the EC identifier, 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. Such modification can therefore only be made by ECHA, which has established a process allowing registrants to adapt the EC identifier initially indicated in the IUCLID dossier when it is not correctly describing the identity of the registered substance. In order to allow such modification of the dossier, the Registrant shall submit a request through the "ECHA Helpdesk contact form", accessible on ECHA's website, at the following link: http://echa.europa.eu/contact/helpdesk-contact-form.

The identifiers adaptation process will apply as follows. This request shall include the chemical name corresponding to the substance that is actually manufactured or imported. If the modification concerns a joint submission involving multiple registrants of the same substance, the adaptation of identifiers requires the agreement in writing on the

modification from every other registrant concerned. Upon receipt of a complete request, ECHA will perform the technical modifications in REACH-IT and will inform the Registrant when the change was performed. The Registrant will then be asked to update the registration dossier with the new identifier.

In order to comply with the present decision pending the completion of the identifier modification process, the Registrant is requested to include the following text 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, but a request has been submitted to ECHA in that respect".

Finally, the Registrant shall ensure that the chemical (IUPAC) name is consistent with the information on the composition reported in IUCLID section 1.2. According to section 4.2.2 of the Guidance for identification and naming of substances for REACH and CLP, only main constituents typically present at ≥10% contribute to the name.

2. Percentage of (significant) main impurities (Annex VI 2.3.3.)

ECHA notes that the registration dossier contains information regarding three impurities present in the registered substance, as required under Annex VI, Section 2.3.3. of the REACH Regulation. The impurities reported in the composition section include one ortho-isomer of tris(methylphenyl) phosphate namely "tris(2-methylphenyl)phosphate". No further ortho-isomer of tris(methylphenyl) phosphate (such as mono- or di-ortho isomers) is reported in the composition section of the IUCLID dossier.

Neither a description of the manufacturing process of the registered substance nor a description of a specific reactivity of the different isomeric forms included in the starting materials was provided in the registration dossier. Lacking such information ECHA assumes that the formation of the possible different isomeric forms of tris(methylphenyl) phosphate follows a statistical distribution. On the basis of such assumption, ECHA considers that mono- or di-ortho isomers are present in the substance in higher concentration levels than the tris-ortho isomer reported in the composition section of the IUCLID dossier.

In addition, ECHA observes that the current concentration values specified in the dossier do not cover 100% of the composition. In particular, the sum of the typical concentrations adds up to [redacted] % (w/w). In line with the Guidance, the composition of well-defined substance should be covered up to 100%. For multi-constituent substances, the sum of typical concentrations for main constituents (≥ 10%) and impurities (< 10%) shall be 100%.

All ortho-isomers of tris(methylphenyl) phosphate (CAS 78-30-8) are subject to harmonised classification. According to Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation), harmonised classification in particular for STOT SE1 classification is triggered at a lower concentration level than 1% (it should be noted that STOT SE2 classification already applies at a concentration limit of 0.2%).

The Registrant shall note that information on the concentration level of the ortho-isomers present in the substance is needed to determine the possible impact of the isomeric composition of the substance on the toxicological properties of the substance.

Furthermore, ECHA notes that, as described in section III 3 and 4 of this decision, the analytical information included in the current registration dossier does not provide any information on how the Registrant determined the concentration levels of the ortho-isomers in the composition of the registered substance in order to conclude on the classification and labelling of the registered substance.

Therefore ECHA concludes that the current compositional information on the contribution of the ortho-isomers of tris(methylphenyl) phosphate, which are expected to be present and are of significance in the determination of the classification and labelling and/or risk assessment of the registered substance, requires further clarification for a unambiguous identification of the substance.

The Registrant is accordingly requested to provide information on the cumulative maximum, minimum and typical concentration values of the ortho-isomers of tris(methylphenyl) phosphate.

Regarding how to report the composition of multi-constituent substances in IUCLID, further technical information is provided in paragraph 2.2.1 of the Data Submission Manual 18 available on the ECHA website.

The Registrant shall ensure that the information provided on the composition of the substance is confirmed by the required analytical data included in IUCLID section 1.4.

3. High-pressure liquid chromatogram or Gas chromatogram (Annex VI, 2.3.6.)

The dossier submitted by the Registrant contains a gas chromatogram (GC), as required by Annex VI Section 2.3.6. However, the GC provided in section 1.4 of the IUCLID dossier is not detailed enough to support the compositional data reported in IUCLID section 1.2.

More specifically, the provided chromatogram presents low resolution. As the peaks shown in the chromatogram are not resolved, it is not clear how the concentration of the constituents (including specific isomeric forms) required to be reported in the registration dossier can be derived. The chromatogram and peak list do not report individual peaks but instead two groups of peaks. Furthermore, the peak list describes the integration for these two groups of peaks and does not report any identification of the peaks with the constituents of the substance reported in IUCLID section 1.2. To correctly identify and quantify the constituents of the substance from the GC data is necessary to resolve, integrate and identify the peaks shown in the chromatogram. Therefore it is not possible to conclude if the GC analytical data provided by the Registrant in IUCLID section 1.4 is in agreement with the compositional information provided in IUCLID section 1.2.

Therefore the Registrant is requested to provide a high-pressure liquid chromatogram (HPLC) or gas chromatogram (GC), including a peak list with the corresponding retention time and peak area.

As for the reporting of the chromatographic data in the dossier, the information shall be attached in IUCLID section 1.4.

The Registrant shall ensure that the description of the analytical method used for the chromatographic analysis, including the experimental set-up (i.e. the column type, length and diameter; injection volume; mobile phase/carrier gas; GC temperature programme; flow rate; concentrations of HPLC standard solutions; detection technique; and run time)

and preparation of solutions and identity of standards, is specified, in line with the requirements of Annex VI section 2.3.7. The Registrant shall ensure that the information is consistent throughout the dossier.

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

ECHA observes that the Registrant did not provide any detailed description of the analytical method used for the identification and quantification of the different constituents present in the composition of the registered substance, which is requested according to Annex VI section 2.3.7.

Although a report of a GC analysis has been provided in the registration dossier, the Registrant did not provide a description of the method used to translate the results of such analysis to the compositional data reported in IUCLID section 1.2. In addition, considering the quality of the chromatogram provided, it is not clear how the quantification of the main constituents and impurities could be carried out (see section II 2.).

Consequently, ECHA notes that the compositional information reported in the registration dossier is not supported by adequate analytical data and therefore the identification and quantification of the registered substance could not be confirmed.

The Registrant is requested to provide a description of the analytical methods used to identify and quantify all the constituents (including all the isomeric forms) required to be reported in the registration dossier. ECHA underlines that the compositional information reported in IUCLID Section 1.2. shall be consistent with those provided in IUCLID Section 1.4.

As for the reporting of the data in the registration dossier, the information shall be attached in IUCLID section 1.4. The information shall be sufficient for the methods to be reproduced and shall therefore include complete details of the experimental protocol followed, the 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/regulations/appeals. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

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