EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000005483-73-03/F Helsinki, 17 November 2014

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

For tert-butyl acetate, CAS No 540-88-5 (EC No 208-760-7), 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 tert-butyl acetate, CAS No 540-88-5 (EC No 208-760-7), submitted by [redacted] (Registrant).

This decision is based on the registration as submitted with submission number [redacted] for the tonnage band 100 to 1000 tonnes per year. This decision does not take into account any updates submitted after 24 July 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 12 September 2013.

On 11 April 2014 ECHA sent the draft decision to the Registrant and invited him to provide comments within 30 days of the receipt of the draft decision. That draft decision was based on submission number [redacted]

On 12 May 2014 ECHA received comments from the Registrant on the draft decision. In addition, on 12 May 2014 the Registrant updated his registration dossier with the submission number [redacted]

The ECHA Secretariat considered the Registrant's comments and update. The information is reflected in the Statement of Reasons (Section III).

On 24 July 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

A. Information in the technical dossier derived from the application of Annexes VII to XI

Pursuant to Articles 41(1), 41(3), 10(a)(vi) and/or (vii), 12(1)(c), 13 and Annex IX of the REACH Regulation the Registrant shall submit the following information using the indicated test methods and the registered substance subject to the present decision:

1. Simulation testing on ultimate degradation in surface water (Annex IX, 9.2.1.2.; test method: Aerobic mineralisation in surface water – simulation biodegradation test, EU C.25./OECD 309) at a temperature of 12°C, as specified in Section III.A.1 below;

2. Identification of degradation products (Annex IX, 9.2.3.) as specified in Section III. A.2 below.

   Note for consideration by the Registrant:

   The Registrant may adapt the testing requested above according to the specific rules outlined in Annexes VI to X and/or according to the general rules contained in Annex XI of the REACH Regulation. In order to ensure compliance with the respective information requirement, any such adaptation will need to have a scientific justification, referring to and conforming with the appropriate rules in the respective Annex, and an adequate and reliable documentation.

   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 the Member States.

B. Information related to chemical safety assessment and chemical safety report

Pursuant to Articles 41(1), 41(3), 10(b), 14 and Annex I of the REACH Regulation the Registrant shall submit in the chemical safety report:

3. Environmental exposure assessment and risk characterisation (Annex I, section 5 and section 6 of the REACH Regulation).

4. Revised exposure and risk assessment for dermal route (Annex I, section 5.2.4. and section 6)

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 **24 May 2016**.

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.

A. Information in the technical dossier derived from the application of Annexes VII to XI

Pursuant to Articles 10(a)(vi) and/or (vii), 12(1)(c) of the REACH Regulation, a technical dossier for a substance manufactured or imported by the Registrant in quantities of 100 to 1000 tonnes per year shall contain as a minimum the information specified in Annexes [VII to IX of the REACH Regulation.

1. Simulation testing on ultimate degradation in surface water (Annex IX, 9.2.1.2.)

"Simulation testing on ultimate degradation in surface water" is a standard information requirement as laid down in Annex IX, 9.2.1.2 of the REACH Regulation. Column 2 of Section 9.2.1.2 of Annex IX further indicates that the study does not need to be conducted if the substance is highly insoluble in water or if the substance is readily biodegradabl The registrant may also seek to adapt the information requirement pursuant to the general adaptation rules of Annex XI, including exposure based adaptation governed by Section 3 of that Annex. Adequate information on this endpoint needs to be present in the technical dossier for the registered substance to meet this information requirement.

In the registration dossier with submission number [redacted], the Registrant has waived simulation testing on ultimate degradation in water and sediment with the following exposure-based justification: *"In accordance with Annex XI, Section 3 of the REACH Regulation (as amended by Regulation 134/2009), further testing of biodegradation in water (including simulation testing) can be waived if absence of significant exposure is demonstrated in the relevant Chemical Safety Report (CSR). Based on information available at the time of the 2010 registration deadline (including legal opinion made available by industry), evaluation of environmental exposure via the generation of exposure scenarios was not judged necessary for substances like that here registered which are not classified in respect of hazard to the environment. For this reason, no detailed evaluation of possible environmental release and exposure was undertaken. Following an ECHA draft CCH decision the registrant has undertaken to prepare a revised CSR for submission including this information. However existing knowledge of the properties and intended uses makes it wholly predictable that CSR revision will lead to a conclusion of low concentration in surface waters, giving rise to no immediate concern for adverse effects on aquatic organisms or health effects via secondary exposure. This conclusion is based on:*
- intended use pattern. Supported uses are restricted to industrial and professional users: as documented in the already submitted CSR, professional use is limited to application of coatings (use resulting in inclusion into/onto a matrix) and small quantity use within laboratories. Hence no wide, dispersive use leading to significant release to wastewater can be expected, so the potential for release into surface waters is very limited
- rapid removal of test substance from aqueous solution via volatilisation. With a vapour pressure of 5599.5 Pa at 20°C, water solubility of 7820 mg/l at 23°C and a Henry's Law Constant of 83.2 Pa-m3/mole (VP/water sol calculated value: the EPISuite v4.11 QSAR programme cites a closely similar experimental database value of 87.3 Pa-m3/mole), modelling by EPISuite leads to very short predicted half-lives in water due to loss by volatilisation: 1.8h in river water, 4.6 days in lake water. These model calculations are confirmed by experimental data: tests using GC analysis of aqueous solutions showed 65-77% loss of test substance via volatilisation from water over 48h at 95-955 mg/l, and total or near-total total loss over 96h at 1070 mg/l."

Furthermore, the Registrant states in his comments on the draft decision: "*In accordance with Annex XI, Section 3 of the REACH Regulation (as amended by Regulation 134/2009), further testing of biodegradation in water of the type proposed in ECHA's draft decision can be waived if absence of significant exposure is demonstrated.*"

ECHA notes that an environmental exposure assessment is not currently provided in the registration dossier. Annex XI, 3.2 of the REACH Regulation states "*The justification shall be based on a thorough and rigorous exposure assessment in accordance with section 5 of Annex I and...*" It is therefore not sufficient to assume 'low exposure' or the absence of wide dispersive uses, but the absence or no significant exposure needs to be demonstrated with an exposure assessment. In the absence of an exposure scenario, the Registrant did not demonstrate the absence of exposure or no significant exposure. The Registrant refers to exposure modelling results included in the registration dossier in their comments on the draft decision. However, the distribution modelling results included in Section 5.4.3 of the registration dossier indicate that under certain modelled conditions a relatively small, but not insignificant fraction of the registered substance ends up in the water compartment. For the Level III analysis, it is stated in the registration dossier that "*Emission to water: Less than 60% tertiary butyl acetate evaporates and is removed by advection. 13% reacts in water and 27% flows downstream. Little transfer to sediment occurs due to the low sorption coefficient of tertiary butyl acetate.*"

Therefore, this waiving statement cannot currently be used as grounds for waiving simulation testing on ultimate degradation in water in accordance with Annex XI, Section 3 of the REACH Regulation.

ECHA also considers that the Registrant has not provided any valid justification to adapt the information requirement for simulation testing in surface water in accordance with the adaptation criteria set out in Column 2 of Annex IX, section 9.2.

ECHA considers that, based on information provided in the registration dossier, the registered substance is not readily biodegradable. According to the technical dossier and the chemical safety report chapters 4.1 and 8.1 the registered substance was identified to be hydrolytically stable with hydrolysis half-life of 6-12 months and based on the chemical structure the Registrant states that it is likely to hydrolyse to tertiary butyl alcohol and acetic acid. However, no analytical data on hydrolysis products is presented. Based on 50 % degradation in ready biodegradability test (OECD 301D) the registered substance cannot be concluded as readily biodegradable. Indeed, when OECD 301D is applied, the threshold for ready biodegradability is 60% in 28 days fulfilling the 10-day window (ECHA Guidance on information requirements and chemical safety assessment, Volume 5 Chapter R7b (November 2012)). The Registrant concludes that the registered substance is partially degraded and it may be inherently biodegradable. Furthermore, the registered substance was not considered to be PBT or vPvB based on the potential inherent biodegradability of the registered substance.

This information shows that the substance is in fact not readily biodegradable within the meaning of Column 2 of Section 9.2.1.2 of Annex IX. In his comments on the draft decision, the Registrant agrees that the substance does not meet the criteria for ready biodegradability but proposes that the data shows evidence of inherent biodegradability. However, ECHA is of the opinion that results of the OECD 301D test reported in the registration dossier do not prove inherent biodegradability since the 50% biodegradation observed in 28 days is significantly less than the pass criterion of 60%.

ECHA considers that the substance cannot be considered as highly insoluble within the meaning of Column 2 of Section 9.2.1.2 of Annex IX since the measured water solubility is reported as 7.8 g/l.

The Registrant has therefore not provided any valid justification to adapt the information requirement for simulation testing in surface water in accordance with the adaptation criteria set out in Column 2 of Annex IX, section 9.2.

For the above reasons, the justification for waiving provided by the Registrant does not meet the criteria of the adaptation rules of either Annex XI, Section 3 of the REACH Regulation or of Column 2 of Annex IX, section 9.2. Therefore, the information available on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently there is an information gap and it is necessary to provide information for this endpoint.

One of the purposes of the simulation test(s) is to provide the information that must be considered for assessing the P/vP properties of the registered substance in accordance with Annex XIII of REACH regulation to decide whether it is persistent in the environment. Annex XIII also indicates that "*the information used for the purposes of assessment of the PBT/vPvB properties shall be based on data obtained under relevant conditions*". The Guidance on information requirements and chemical safety assessment R.7b (version 1.2, November 2012) specifies that simulation tests "attempt to simulate degradation in a specific environment by use of indigenous biomass, media, relevant solids [...], and a typical temperature that represents the particular environment". The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation., Table R.16-9 (version 2.1 October 2012) indicates 12 °C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment.

ECHA considers that performing the test(s) at the temperature of 12 °C is within the applicable test conditions of the Test Guideline OECD 309.

As for the applicability of the OECD guideline to this volatile substance, ECHA notes that the OECD TG 309 foresees testing of "*slightly volatile*" substances. Paragraph 7 of the OECD TG 309 further clarifies: "*Using closed flasks with a headspace, it is possible to test slightly volatile substance (with Henry's law constants <100 Pa · m3/mol or <10-3 atm · m3/mol) without losses from the test system*". As the Registrant indicates in his comments, the registered substance has a vapour pressure of 5599.5 Pa at 20°C, water solubility of 7820 mg/l at 23°C and a Henry's Law Constant of 83.2 Pa-m3/mole (VP/water solubility calculated value; EPISuite v4.11 cites an experimental database value of 87.3 Pa-m3/mole). Thus, the Henry's Law Constant falls within the range indicated as being possible to test according to OECD TG 309. The Registrant shall therefore take into account the substance properties (volatility) when performing the test.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the following information derived with the registered substance subject to the present decision:

> Simulation testing on ultimate degradation in surface water (Annex IX, 9.2.1.2.; test method: Aerobic mineralisation in surface water – simulation biodegradation test (test method: EU C.25./OECD 309) at a temperature of 12 °C.

Note for the Registrant

Before conducting the test mentioned above the Registrant is advised to consult the ECHA Guidance on information requirements and chemical safety assessment (version 1.2, November 2012), Chapter R7b, Sections R.7.9.4 and R.7.9.6 and Chapter R.11.1.3 on PBT assessment.

In accordance with Annex I, Section 4, of the REACH Regulation the Registrant should revise the PBT assessment when results of the test detailed above is available. The Registrant is also advised to consult the ECHA Guidance on information requirements and chemical safety assessment (version 1.1, November 2012), Chapter R.11.1.3. and Figure R. 11-1 on PBT assessment for the integrated testing strategy for persistency assessment in particular taking into account the degradation products of the registered substance.

2. Identification of degradation products (Annex IX, 9.2.3.).

The identification of the degradation products is a standard information requirement according to column 1, Section 9.2.3 of Annex IX of the REACH Regulation. Column 2 of Section 9.2.3. of Annex IX further states that the study does not need to be conducted if the substance is readily biodegradable.

The technical dossier contains the following information related to the standard information requirement to identify degradation products pursuant to Annex IX, 9.2.3. Based on 50 % degradation in 28 days in an OECD 301D ready biodegradation test, the Registrant concludes that the registered substance is inherently biodegradable. The Registrant does not report information on potential degradation products or their fate. Hydrolysis studies conducted according to OECD 111 results in a hydrolysis half-life of 6 -12 months under environmental conditions. Based on the chemical structure of the registered substance,the Registrant considered that potential hydrolysis products would be tertiary butyl alcohol and acetic acid. ECHA notes that no data was provided to support this assumption.

As dicussed above, the Registrant concludes that the substance is not readily biodegradadable. ECHA notes that the results in the technical dossier indicate that the substance is not fully degraded or mineralised and the identification of degradation products is missing. Therefore the adaptation of Column 2 of Section 9.2.3 of Annex IX cannot be applied. The Registrant has neither presented any valid adaptation within the meaning of Annex XI in his dossier.

As explained above, the information available on this endpoint for the registered substance in the technical dossier does not meet the information requirement. Consequently there is an information gap and it is necessary to provide information for this endpoint.

Regarding an appropriate and suitable test method, the methods will have to be substance specific. When analytically possible, identification, stability, behaviour, molar quantity of metabolites relative to the parent compound shoud be evaluated.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the following information derived with the registered substance subject to the present decision:

Identification of the degradation products using an appropriate and suitable test method, as explained above in this section.

Note for the Registrant

Before conducting the identification of the degradation products the Registrant is advised to consult the ECHA Guidance on information requirements and chemical safety assessment Chapter R.7b (version 1.2, November 2012), Sections R.7.9.2.3 and R.7.9.4. These guidance documents explain that the data on degradation products is only required if information on the degradation products following primary degradation is required in order to complete the chemical safety assessment. Section R.7.9.4. further states that when substance is not fully degraded or mineralised, degradation products may be determined by chemical analysis.

In accordance with Annex I, Section 4 of the REACH Regulation, the Registrant should revise his PBT assessment when results of the test detailed above are available. The Registrant is also advised to consult ECHA Guidance on information requirements and chemical safety assessment R.11 (version 1.1, November 2012), Chapter R.11.1.3 and Figure R.11-1 on PBT assessment for the integrated testing strategy for persistency assessment in particular taking into account the degradation products of the registered substance.

In addition, degradation half-life, log Kow and potential toxicity of the degradation products may be investigated. The Guidance on information requirements and chemical safety assessment Chapter R.16 on Environmental Exposure Estimation., Table R.16-9 (version 2.1 October 2012) indicates 12 °C (285K) as the average environmental temperature for the EU to be used in the chemical safety assessment.

B. Information related to the chemical safety assessment and chemical safety report

3. Environmental exposure assessment and risk characterisation (Annex I, section 5 and section 6 of the REACH Regulation).

Annex I, section 5 of the REACH Regulation requires the Registrant to generate exposure scenarios and exposure estimations for the registered substance. The exposure assessment shall consider, in the exposure assessment, all stages of the life-cycle of the substance resulting from the manufacture and identified uses and shall cover any exposures that may relate to the identified hazards.

Annex I, section 6 of the REACH Regulation requires the Registrant to characterise the risk for each exposure scenario and shall consider the human population (exposed as workers, consumer or indirectly via the environment and if relevant a combination thereof) and the environmental spheres for which exposure to the substance is known or reasonable foreseeable, under the assumption that the risk management measures described under exposure scenario in the section 5 have been implemented. In addition, the overall environmental risk caused by the substance shall be reviewed by integrating the results for the overall releases, emissions and losses from all sources to all environmental compartments.

In the chemical safety report (CSR) provided by the Registrant the exposure assessment for the environment is missing. The Registrant claims that no exposure assessment is necessary for the environment by stating that "As a result of the hazard assessment carried out in accordance to article 14.3, the registrant concludes that the substance does not meet the criteria for classification as dangerous for the environment; therefore risk characterisations for environmental endpoints were not developed."

ECHA notes that the Registrant has classified the substance as "Flam. Liquid 2 H225: Highly flammable liquid and vapour" (GHS) and "F; R11 Highly flammable" (DSD) and thus, fulfilling the criteria set out in Article 14(4) of the REACH Regulation to require an exposure assessment and a risk characterisation in the chemical safety assessment. In addition, hazards have also been identified in the environmental studies submitted in the registration dossier.

With regard to the scope of the required exposure assessment, as stated above and in accordance with Annex I, 5.0., it has to cover all hazards that have been identified according to Sections 1 to 4 of Annex I of the REACH Regulation.

In his comments on the draft decision, the Registrant agreed to the request to perform an environmental exposure and risk assessment for the registered substance. The Registrant also confirmed in the comments that their supported uses of the registered substance are restricted to industrial and professional users and consumer uses are not supported.

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation of the REACH Regulation, the Registrant is requested to generate an exposure assessment and risk characterisation for the environment. The chemical safety report shall be amended accordingly.

4. Revised exposure and risk assessment for dermal route (Annex I, section 5.2.4. and section 6)

Pursuant to sections 0.6.2. and 0.6.3. of Annex I of the REACH Regulation the chemical safety assessment (CSA) performed by a Registrant shall include an exposure assessment according to section 5 of Annex I. Annex I, section 5.2.4. of the REACH Regulation, requires the Registrant to perform an estimation of the exposure levels for all human populations (workers, consumer and humans liable to exposure via the environment) for which exposure to the substance is known or reasonably foreseeable. Each relevant route of exposure (inhalation, oral, dermal and combined through all relevant routes and sources of exposure) shall be addressed. In addition, Annex I, section 5.2.5. of the REACH Regulation indicates that appropriate models can be used for the estimation of exposure levels. Section 6 of the CSR requires the Registrant to carry out a risk characterisation for each exposure scenario.

ECHA notes that the Registrant has used ECETOC TRA version 2 to estimate exposure for a variety of worker and consumer exposure scenarios. More specifically the Registrant has used the local exhaust ventilation (LEV) exposure modifier for estimating dermal exposure.

ECHA underlines that the Guidance on information requirements and chemical safety assessment, R.14 version 2.1 (section R.14.4.8, page 21) advises against the use of the LEV modifier for dermal exposure estimation.

ECHA notes that the calculated exposure estimates are therefore likely to be underestimated and accordingly the worker exposure assessment for the dermal route needs to be revised.

As explained above, the information provided on the dermal exposure estimates for the registered substance in the CSR does not meet the general provisions for preparing a CSR as described in Annex I. Consequently it is necessary to revise the dermal exposure estimates.

Based on the above the Registrant shall revise the exposure assessment for dermal route and assess related risks. The Registrant shall ensure that the calculated risk characterisation ratios will still be below 1, in order to demonstrate the safe use of the registered substance. The CSR shall be amended accordingly.

IV. Adequate identification of the composition of the tested material

In carrying out the studies required by the present decision it is important to ensure that the particular sample of substance tested is appropriate to assess the properties of the registered substance, taking into account any variation in the composition of the technical grade of the substance as actually manufactured. If the registration of the substance covers different grades, the sample used for the new studies must be suitable to assess these.

Furthermore, there must be adequate information on substance identity for the sample tested and the grade(s) registered to enable the relevance of the studies to be assessed.

V. 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://www.echa.europa.eu/web/guest/regulations/appeals. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

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Director of Evaluation
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