EUROPEAN CHEMICALS AGENCY

~~HIGHLY RESTRICTED~~

Decision number: CCH-D-0000004607-70-03/F Helsinki, 23 June 2014

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

For Phenol, dodecyl-, branched, CAS No 121158-58-5 (EC No 310-154-3), 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 Phenol, dodecyl-, branched, CAS No 121158-58-5 (EC No 310-154-3), submitted by [redacted] (Registrant).

This decision is based on the registration as submitted with submission number [redacted], for the tonnage band of 1000 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 2 September 2013.

On 17 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 16 January 2014 ECHA received comments from the Registrant on the draft decision.

The ECHA Secretariat considered the Registrant's comments and, as the comments did not contain new information related to the concerns raised in this decision, did not 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

A. 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, 2.1.);
2. Composition of the substance (Annex VI, 2.3.)

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

Pursuant to Articles 41(1)(a), 41(3), 10(a)(vi) and/or (vii), 12(1)(e), 13 and Annexes VII, VIII, IX, X of the REACH Regulation the Registrant shall submit the information on test material identity to complete the robust study summaries as defined by Article 3(28) and detailed in the Practical Guide 3: How to report robust study summaries[1] on the following endpoints:

1. Ready biodegradability (Annex VII, 9.2.1.1.)
2. Bioaccumulation in aquatic species (Annex IX, 9.3.2.)
3. Adsorption/desorption screening (Annex VIII, 9.3.1.)
4. Short-term toxicity testing on fish (Annex VIII, 9.1.3.)
5. Short-term toxicity testing on aquatic invertebrates (Annex VII, 9.1.1.)
6. Long-term toxicity testing on aquatic invertebrates (Annex IX, 9.1.5.)
7. Growth inhibition study aquatic plants (Annex VII, 9.1.2.)
8. Activated sludge respiration inhibition testing (Annex VIII, 9.1.4.)
9. Acute toxicity by oral route (Annex VII, 8.5.1.)
10. Acute toxicity by dermal route (Annex VIII, 8.5.3.)
11. *In vivo* skin irritation (Annex VIII, 8.1.1.)
12. *In vivo* eye irritation (Annex VIII, 8.2.1.)
13. Skin sensitisation (Annex VII, 8.3.)
14. Short-term repeated dose toxicity study (28 days), oral route (Annex VIII, 8.6.1.)
15. Sub-chronic toxicity study (90-day), oral route (Annex IX, 8.6.2.)
16. *In vitro* gene mutation study in bacteria (Annex VII, 8.4.1.)
17. *In vitro* gene mutation study in mammalian cells (Annex VIII, 8.4.3.)
18. *In vivo* mammalian erythrocyte micronucleus test (Annex IX/X, 8.4., column 2)
19. Two-generation reproductive toxicity study (Annex [IX/X], 8.7.3.)
20. Pre-natal developmental toxicity study (Annex IX, 8.7.2.)

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 **30 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.

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

A. 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)

"Name or other identifier of the substance" is an information requirement as laid down in Annex VI, Section 2.1 of the REACH Regulation. 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 technical dossier for the registered substance to meet this information requirement.

ECHA notes that the Registrant identified the registered substance as of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB).Information required to be provided on the naming of UVCB substances such as the registered substance shall consist of two parts: (1) the chemical name and (2) a more detailed description of the manufacturing process, as indicated in chapter 4.3 of the Guidance for identification and naming of substances under REACH and CLP (Version: 1.2, March 2012) - referred to as "the Guidance" thereinafter. ECHA observes that the Registrant did not provide sufficient information on the naming of the registered substance (as indicated in point (i) and (ii) thereinafter).

(i). Chemical name

The Registrant assigned, as chemical name for the registered substance in the IUPAC name field in IUCLID section 1.1, "*phenol, alkyl branched (species comprising decyl, undecyl, dodecyl, tridecyl, tetradecyl, pentadecyl, substituents)*". Whilst this chemical name designates, in generic terms, six different groups of branched alkyl phenol constituents which are also reported by the Registrant in the composition, it does not accurately reflect the identity and predominance of the constituents actually present in the composition of the manufactured substance. In particular, according to the compositional information reported in IUCLID section 1.2, the C9 (branched) alkylphenols which are not quoted in the name can be present at a higher concentration level (up to [redacted] %(w/w)) than the C15 (branched) alkylphenols quoted in the name and for which the contribution does not exceed [redacted] %(w/w)). In addition, the current chemical name reported in the IUPAC name field in IUCLID section 1.1 does not specify the position of the branched alkyl substituents on the aromatic ring of these phenol derivatives.

ECHA observes that the Registrant recognised, in the description field of the reference substance in IUCLID section 1.1, that "*[a] more meaningful name to describe this UVCB substance*" could be provided and suggested for that purpose "*phenol, alkylation products with C10-C15 branched olefins derived from propene oligomerisation*". However, the suggested alternative chemical name does not specify the position of the alkyl substituent, nor does it provide a representative carbon number range for the branched alkyl substituent (as already explained above).

ECHA therefore concludes that the Registrant did not provide a representative chemical name for the registered substance.

The Registrant is accordingly required to revise the chemical name assigned to the registered substance as specified in the first bullet point of sub-section (iii) below.

(ii). The manufacturing process

ECHA observes that the Registrant provided a generic description of the manufacturing process in section 3.1 of the IUCLID dossier. According to this description, the registered UVCB substance is manufactured by reacting phenol and an olefin under catalytic conditions and purifying the product from this reaction by a distillation step to remove "impurities". However, this generic description is not considered sufficient to identify the registered substance, as explained thereinafter.

The analytical information currently provided by the Registrant in IUCLID section 1.4 of the dossier indicates that the registered substance consists of the following:

- A complex set of phenol-based constituents with an alkyl branched structure of carbon number varying from below C9 (referred to as "light alkylphenols" by the Registrant) up to at least C15. These alkyl substituents can be both in ortho- and para- position on the phenol ring;
- Other groups of constituents such as unreacted starting materials, dialkyl ethers and dialkylphenols.

The composition of the registered substance is therefore expected to consist of a large number of constituents. As a result of the complexity in the composition, the registered UVCB substance can normally not be fully identified on the basis of its chemical composition alone without further detail on the manufacturing process, as explained in chapter 4.3 of the Guidance. The manufacturing process description to be provided shall normally consist of the chemical identity and ratio of the starting materials actually used and information on the most relevant steps of the manufacturing process and the associated process parameters, as also specified in chapter 4.3 of the Guidance. However, the Registrant did not specify the following information:

- The ratio of reactants used in the process. This information may determine the level of alkylation of the phenol in the manufactured substance. The alkylation level however can currently not be derived from the reported composition, in line with the observations in section III.1.2 of this decision;
- Sufficient details on the composition of the olefin used, in particular the contribution of the "light" olefins ending up as "light alkylphenols" mentioned in the analytical reports. This contribution can currently not be derived from the composition reported in the dossier, in line with the observations in section III.1.2 of this decision;
- Further information on the processing steps and processing parameters, such as the catalysis type, determining the relative abundance of para-alkylphenol constituents over the ortho-alkyl constituents. The information on the relative abundance of these groups of constituents is currently limited to a quantification carried out on the analysed sample in IUCLID section 1.4.
- Further description of the distillation step, more specifically the fraction of the distillation step from which the registered substance is isolated. This information determines the constituents within the reaction products (light fraction and/or heavy fraction - distillation residues) for which the contribution in the composition of the manufactured substance is minimised. This information can currently not be derived from the reported composition, in line with the observations in section III.1.2 of this decision.

The Registrant is accordingly required to provide the missing information on the manufacturing process description, as specified under the second bullet point of sub-section (iii) below.

(iii). The information required from the Registrant

- A chemical name representative of the registered substance must be provided.

  Based on the observation set out in sub-section (i) above, the Registrant is required to revise the chemical name currently assigned to the registered substance. The chemical name shall reflect the identity (including the carbon number distribution) of the branched alkyl substituents as well as their position on the aromatic ring of the phenol constituents of the registered substance. Taking into account the following observations in the registration dossier:

  - The declaration from the Registrant, in the Description field in IUCLID section 1.1, that the olefin starting material used in the process is characterised by the relative predominance of C12 olefin constituents,

  - The indication that the substance predominantly consists of para-alkylphenol isomers (i.e. the para-alkylphenol isomers represent ≥80%(w/w)), as suggested by the results from analyses reported in IUCLID section 1.4,

  ECHA considers that, under these specific circumstances, "Phenol, *para*-alkylation products with C12-rich branched olefins from propene oligomerisation" is an appropriate chemical name for the registered substance.

- Further detail on the manufacturing process must be provided

  Based on the observation set out in sub-section (ii) above and pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant shall specify the following information on the manufacturing process:

  - Ratio of reactants;
  - the overall composition of the olefin starting material, including the identity and upper and lower concentration levels of the olefins presenting the same carbon number and ending up as light alkylphenols in the registered substance;
  - Description of the processing steps and processing parameters which determine the relative abundance of para-alkylphenol constituents over the ortho-alkyl constituents;
  - Identification of the fraction of the distillation step from which the registered substance is isolated.

The Registrant shall ensure that the information is consistent throughout the dossier.

Regarding how to report the manufacturing process, the chemical name and manufacturing process description shall be specified in the "IUPAC name" and "Description" fields in IUCLID section 1.1, respectively.

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

"Composition of the substance" is an information requirement as laid down in Annex VI, Section 2.3. of the REACH Regulation. 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 cornerstone of all the REACH obligations. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the composition reported in section 1.2 of the IUCLID dossier is not described to a sufficient level of detail and is not consistent with the information provided on composition in the analytical report attached in IUCLID section 1.4 of the registration dossier.

More specifically, the Registrant reported, in IUCLID section 1.2 of the registration dossier, seven groups of mono-(branched alkyl)-substituted phenol constituents which differ from each other in terms of the carbon number of the branched alkyl group (from C9 to C15). ECHA observes that the reported composition does not provide any further information on the position of these branched alkyl groups on the phenol ring. ECHA however notes that, in the analytical report attached in section 1.4, the Registrant provided a description of analytical methods for the quantification of the *ortho*- and *para*-branched alkyl phenols. ECHA therefore concludes that the current composition has not been provided to a sufficient level of detail.
In addition, the typical breakdown of the composition currently reported in IUCLID section 1.2 would indicate that the registered substance exclusively consists of mono-(branched alkyl)-substituted phenol constituents, the typical concentration of these seven groups of constituents adding up to 100% (w/w). However, in the analytical report attached in IUCLID section 1.4, the Registrant provided a description of analytical methods for the quantification of other constituents including the unreacted starting material, [redacted]. ECHA therefore concludes that the concentration levels currently reported in the composition are not consistent with the conclusions from the analytical report attached to the dossier and that the constituents and groups of constituents required to be reported have not all been accounted for in the composition.

According to chapter 4.3 of the Guidance, the Registrant shall note that, for UVCB substances such as the registered substance, the following applies:

- All constituents present in the substance with a concentration of ≥ 10 % shall be identified and reported individually;
- All known constituents and constituents relevant for the classification and/or PBT assessment of the registered substance shall be reported individually; and
- Unknown constituents or groups of constituents shall be identified as far as possible by a generic description of their chemical nature.

For each constituent and group of constituents, the minimum, maximum and typical concentration, shall be reported.

Pursuant to Article 41(1)(a) and (3) of the REACH Regulation, the Registrant is accordingly requested to specify, for each (branched alkyl)phenol group constituents presenting the same carbon number, the relative contribution in *ortho*- and *para*- isomers in the form of a range reflecting the variability observed in the composition and to report the known constituents or groups of constituents which have not been reported in composition.

The Registrant shall ensure that the information is consistent throughout the dossier.

Regarding how to report the composition in IUCLID, the following applies: The Registrant shall indicate the composition of the registered substance 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. For the other constituents to be reported under a generic description, a generic chemical name describing the group of constituents, generic molecular and structural information (if applicable), as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID. Regarding the reporting of the contribution of the ortho- and para- isomers of the alkylphenols already specified in the composition, the Registrant shall indicate the contribution of these groups of isomers in the Remarks field of the repeatable block for each reported alkylphenol in the form range, such as "para-/ortho- ratio varies from [minimal ratio] to [maximal ratio]".

Further technical details on how to report the composition of UVCB substances in IUCLID are available in paragraphs 2.1 and 2.2.2 of 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.

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

Pursuant to Articles 10(a)(vii), 12(1)(e) of the REACH Regulation, a technical dossier for a substance manufactured or imported by the Registrant in quantities of 1000 tonnes or more per year shall contain as a minimum the information specified in Annexes VII, VIII, IX, and X of the REACH Regulation. The technical dossier shall include robust study summaries for the information derived from application of Annex VII-X. A robust study summary is defined as "detailed *summary of objectives, methods, results and conclusions of a full study report providing sufficient information to make an independent assessment of the study minimising the need to consult the full study report*" (Article 3(28)).

The submitted technical dossier does not provide sufficient information to make an independent assessment of the studies possible for the following endpoints missing the information on test material identity given below:

1. Ready biodegradability (Annex VII, 9.2.1.1.)
2. Bioaccumulation in aquatic species (Annex IX, 9.3.2.)
3. Adsorption/desorption screening (Annex VIII, 9.3.1.)
4. Short-term toxicity testing on fish (Annex VIII, 9.1.3.)
5. Short-term toxicity testing on aquatic invertebrates (Annex VII, 9.1.1.)
6. Long-term toxicity testing on aquatic invertebrates (Annex IX, 9.1.5.)
7. Growth inhibition study aquatic plants (Annex VII, 9.1.2.)
8. Activated sludge respiration inhibition testing (Annex VIII, 9.1.4.)
9. Acute toxicity by oral route (Annex VII, 8.5.1.)
10. Acute toxicity by dermal route (Annex VIII, 8.5.3.)
11. *In vivo* skin irritation (Annex VIII, 8.1.1.)
12. *In vivo* eye irritation (Annex VIII, 8.2.1.)
13. Skin sensitisation (Annex VII, 8.3.)
14. Short-term repeated dose toxicity study (28 days), oral route (Annex VIII, 8.6.1.)

15. Sub-chronic toxicity study (90-day), oral route (Annex IX, 8.6.2.)
16. *In vitro* gene mutation study in bacteria (Annex VII, 8.4.1.)
17. *In vitro* gene mutation study in mammalian cells (Annex VIII, 8.4.3.)
18. *In vivo* mammalian erythrocyte micronucleus test (Annex IX/X, 8.4., column 2)
19. Two-generation reproductive toxicity study (Annex [IX/X], 8.7.3.)
20. Pre-natal developmental toxicity study (Annex IX, 8.7.2.)

In relation to the information required by the present decision, the registrant needs to demonstrate that the test material used for the studies must be suitable for use by all the joint registrants. Hence, it needs to be demonstrated that the sample used had a composition that is within the specifications of the substance composition that are given by the registrant and other joint registrants. It is the responsibility of all joint registrants who manufacture or import the same substance to agree on the appropriate composition of the test material and to document the necessary information on their substance composition.

In addition, it is important to demonstrate that the particular sample of substance tested in the studies 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 by each registrant. If the registration of the substance by any registrant covers different grades, the sample used for the new studies must be suitable to assess these grades.

Finally 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.

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/appeals/app_procedure_en.asp. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

[redacted]
Leena Ylä-Mononen
Director of Evaluation

Annex I: Practical Guide 3. How to report robust study summaries
echa.europa.eu/documents/10162/13643/pg_report_robust_study_summaries_en.pdf