ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114308163-62-01/F Helsinki, 2 September 2015

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

For Phenol, dodecyl-, sulfurized, calcium salts, CAS No 68855-45-8 (EC No 272-486-4), 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-, sulfurized, calcium salts, CAS No 68855-45-8 (EC No 272-486-4), 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 23 July 2015, 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 2016.

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 1 October 2013.

On 25 September 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 31 October 2014 ECHA received comments from the Registrant on the draft decision.

On 26 November 2014 the Registrant updated his registration with the submission number [redacted].

The ECHA Secretariat considered the Registrant's comments and update.
On basis of this information, Section II was amended. The Statement of Reasons (Section III) was changed accordingly.

On 23 July 2015 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, 2.1.);
2. The description of the analytical methods (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 **9 December 2015**.

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.)

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 according to Annex VI section 2.1 of the REACH Regulation on the naming of UVCB substances such as the registered substance shall consist of two parts: the chemical name and 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: 1.3, February 2014) - referred to as "the Guidance" thereinafter. ECHA observes that the Registrant did not provide sufficient information on the naming of the registered substance (as explained under points (i) and (ii) thereinafter).

(i). The chemical name and numerical identifiers used in the dossier do not correspond to other information reported in IUCLID section 1 of the registration dossier.

The chemical name originally specified by the Registrant for the registered substance, which is also the chemical name associated with the EC entry (EC No

272-486-4) and CAS entry (CAS No 68855-45-8) assigned in the original dossier, indicated that the registered substance was a derivative of "phenol, dodecyl-", i.e. of a phenol including a linear C12 alkyl substituent at an undefined position on the aromatic ring. However, in IUCLID sections 1.1 and 1.2 of the original dossier, the Registrant made also reference to the registered substance as a derivative of different alkylphenols than "phenol, dodecyl-", including:

- a derivative of phenol that is alkylated by "*C10 - 15 branched olefins derived from propene oligomerization*", i.e. to a phenol including a branched alkyl substituent at an unspecific position and presenting a carbon number distribution represented by the C10, C11, C12, C13, C14 and C15 carbon numbers.
- a derivative of "phenol, tetrapropylene-" and therefore of an alkylphenol normally expected to have a specific branched C12 alkyl substituent.
- a derivative involving also the residues obtained in the manufacturing of tetrapropenylphenol.

ECHA thus addressed in its initial draft decision the abovementioned inconsistencies identified in the dossier on the naming of the registered substance. ECHA also indicated on how to revise the information on the EC entry, CAS entry and chemical name assigned to the registered substance.

The Registrant revised, in the dossier update following the notification of the draft decision (hereinafter the "update dossier"), the chemical name and CAS information assigned to the registered substance. These identifiers refer to "*Phenol, (tetrapropenyl) derivs., reaction products with distn. residues from manuf. of phenol (tetrapropenyl) derivs. and sulfur, calcium salts*", which is a substance corresponding to calcium salts of reaction products from 3 different starting materials:

- Phenol, (tetrapropenyl) derivatives;
- Distillation residues from the manufacturing of phenol (tetrapropenyl) derivatives;
- Sulfur.

This information is however not consistent with the reported manufacturing process description included in the update dossier. In particular, the manufacturing process description only mentions the use of 2 starting materials, said the "[redacted]" and "[redacted]". No reference is made to the use of "[redacted]" in the manufacturing of the registered substance.

This information is also inconsistent with the EC entry (EC No 272-486-4) currently assigned to the registered substance. This EC entry refers to a UVCB substance obtained from a different phenol derivative (i.e. of "phenol, dodecyl-") than any of those referred to as starting material in the chemical name and CAS information of the update dossier. The Registrant however did not indicate in the update dossier that this EC information does not specifically correspond to the registered substance.

In addition, ECHA observes that the registration update includes further inconsistencies regarding the identity of the phenols starting materials. More specifically, regarding the position of the alkyl substituent on the phenol ring:

- The chemical name and CAS information assigned to the substance in the update dossier suggests that the position is unspecific (and therefore is represented by all 3 possible positions ortho-/meta-/para-).

- Other information also submitted by the Registrant in the update dossier would indicate that the representative position of the alkyl substituent is in fact para-:
  - The reaction schemes included in the manufacturing process attached in IUCLID section 1.4 suggest that both the ortho- and para- isomers are present. The description provided in IUCLID section 1.2 furthermore specifies the predominance of the para- isomers, the reported ratio being "[redacted]% para and [redacted] % ortho".
  - The structural information of the constituents of the registered substance also suggests that the representative position of the alkyl substituent is [redacted]-.

Based on these inconsistences in the updated dossier, ECHA concludes that the chemical name and EC and CAS identifiers currently assigned by the Registrant to the registered substance cannot be considered appropriate for its identification.

(ii). Elements of the manufacturing process description which are essential for the identification of the registered substance are missing from the dossier.

The identity of the alkyl phenol starting material had not been identified to a sufficient level of detail in the original dossier. Other essential elements of the process description were not reported. In particular, The Registrant did not specify the exact ratio of the different reactants used for the manufacturing. Moreover, the Registrant did not define the parameters and the corresponding specifications (as values) used to control the composition of the registered substance, including the degree of sulfurisation and 'oligomerisation' of the alkyl phenolate. Furthermore, no details on the collection and purification steps were provided.

ECHA thus addressed in its initial draft decision the missing information on the manufacturing process description mentioned above (i.e. detailed compositional information of the alkylphenol starting material, ratio of reactants, details of the parameters used to control the composition of the manufactured substance and description of the purification/isolation steps).

The Registrant provided, in the update dossier, specifications of the composition of the alkylphenol starting material used in IUCLID section 1.2. The Registrant also attached, in IUCLID section 1.4, a process description including the process parameters used for the manufacturing, reaction schemes, qualitative information on the level of sulfurization and "oligomerisation", as well as specification of the purification and isolation steps. The Registrant however did not specify the exact ratio of reactants used. Taking into account that the update dossier includes uncertainties on the identity of the starting materials, as mentioned in chapter III.1.(i) of this decision, and on the distribution of the different phenates obtained from the manufacturing (this distribution being expected to be influenced by the ratio of reactants used), as mentioned in chapter III.2 of this decision, ECHA considers that the information on the ratio of reactants is still necessary for the identification of the registered substance.

In line with the observations under point (i), the Registrant is accordingly requested to address the abovementioned inconsistencies identified in the dossier on the naming of the registered substance. Concerning the chemical name, EC number and CAS number currently assigned to the registered substance in IUCLID section 1.1, if this information is not

appropriate for identification of the registered substance, the Registrant shall revise the information as follows:

- The Registrant shall replace the chemical name currently specified by a chemical name that reflects the exact identity of the alkylphenol starting material used and the composition of the registered substance.
- The Registrant shall delete from the dossier the CAS entry currently assigned to the substance and provide instead any available CAS information specifically corresponding to the substance.
- The Registrant shall not 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. To ensure unambiguous identification of the registered substance, the Registrant shall however specify in the dossier that the EC entry currently assigned does not specifically correspond to the registered substance and refer to any available and appropriate EC number specifically corresponding to the substance.

In line with the observations under point (ii), the Registrant shall provide the missing information on the manufacturing process description mentioned above (i.e. the ratio of reactants).

As for the reporting of the information in IUCLID, the chemical name and the manufacturing process description shall be specified in the "IUPAC name" and "Description" fields in IUCLID section 1.1, respectively. Any available CAS information shall be reported under the CAS information header of the reference substance in IUCLID section 1.1. Should the Registrant establish that the EC and CAS information currently assigned does not specifically correspond to the registered substance, the Registrant may report the CAS entry with CAS number 220794-90-1 under the "Related CAS information" header of the reference substance in IUCLID section 1.1. The Registrant shall then specify, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 272-486-4 currently assigned does not specifically correspond to the registered substance. This identifier can technically not be modified or deleted at this stage in the present registration update". The Registrant shall also specify, in the same IUCLID field, any available and appropriate EC number for the substance.

The Registrant shall ensure that the name and other identifiers to be assigned to the registered substance are consistent with each other and with the composition required to be reported according to Annex VI Section 2.3 of the REACH Regulation. The Registrant shall also 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.

2. The description of the analytical methods (Annex VI, 2.3.7.)

The Registrant did not provide, in the original dossier, any description of the analytical method used for the identification of the registered substance, including its constituents, as required by Annex VI, 2.3.7. of the REACH regulation.

In particular, the Registrant attached a copy of an HPLC chromatogram. However, this information was not part of any quantitative analysis of constituents and groups of constituents. Furthermore, the analytical information reported in the dossier did not provide any description of the analytical methods used for the identification and quantification of the constituents required to be reported in the composition.

Regarding the high concentration level of the mineral oil (from [redacted] % (w/w)) reported in the original composition, this oil was presented by the Registrant as acting (also) as a solvent in IULCLID section 1.2. In line with Article 3(1) of the REACH Regulation, the quantity of oil which can be removed without affecting its stability or changing the composition of the registered substance shall be excluded. However, the extent to which the oil could be removed was ambiguous. In particular, it was indicated in IUCLID section 1.4 of the dossier that "attempts to remove this base oil from the substance result in changes to the other components' original structures and the physicochemical characteristics of the substance as a whole. With this in mind, the substance is being registered to include the base oil as a component of the substance and thus the base oil is present in the test material". The fact that the base oil could not be removed from the substance without affecting its properties and stability did not seem to be in line with the information on the test materials used to characterize some of the hazard endpoint data in sections 4-6 of the IUCLID dossier. Tests have indeed been performed with commercial samples reported to have typical concentration in oil of as low as [redacted]%.

ECHA thus addressed in its initial draft decision the description of the analytical methods used for the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance. As the presence of high overall concentration of the constituents from the highly refined oil contributes to the identification of the registered substance, the description of the analytical methods used to determine the extent to which oil can be removed from the substance composition was therefore also requested from the Registrant.

The Registrant attached, in the update dossier, details of the procedures used for recording UV, IR, NMR and MS spectra such as the ones already included in the registration dossier. However, the description of the method for the quantification of the constituents required to be reported is still missing:

- The method used to quantify the unreacted branched dodecylphenol derivatives has not been specified;
- There is no information as to how the Registrant established the presence of the different structures reported for the different phenates obtained (referred to as "dimer", "trimer", "tetramer" and "pentamer" by the Registrant in IUCLID section 1.2);
- The carbon number distribution of the alkyl substituents of the phenates in the composition of the registered substance has not been supported by analytical information.

Concerning the methods for the quantification of the constituents present in the oil originally reported in the composition, ECHA takes note that the Registrant removed the reference to the presence of oil in the composition of the registered substance. This implies that the oil originally reported in the registration does not contribute to the composition of the registered substance. Accordingly, a description of methods for the quantification of the constituents originating from the oil is not required. However, the Registrant still acknowledges the presence of oil in the composition of the sample used for the analyses currently described in the dossier (including the NMR and IR analyses). It is therefore unclear how the oil present in the composition of the analysed sample contributes to the composition of the registered substance.

The Registrant is accordingly requested to provide a description of the analytical methods used for the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance. The Registrant shall

also clarify the origin of the oil present in the composition of the analysed sample and the reason why the oil does not contribute to the composition of the manufactured 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. The information shall be sufficient for ECHA to verify both qualitatively and quantitatively the compositional information required to be specified in the dossier. ECHA would like to underline that, subject to a case-by-case analysis, ECHA will accept any approach that is sufficient to verify the reported composition. Accordingly, the analyses requested are not limited to chemical analyses directly carried out on a sample of the registered substance but can also be based for instance on analyses of the derivatised substance, theoretical calculations and considerations on the manufacturing process conditions.

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

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

Authorised[1] by Claudio Carlon, Head of Unit, Evaluation

[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.