EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-2114309013-68-01/F Helsinki, 30 September 2015

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

For 2,4-Pentanedione, peroxide, CAS No 37187-22-7 (EC No 253-384-9), 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 2,4-Pentanedione, peroxide, CAS No 37187-22-7 (EC No 253-384-9), submitted by [redacted] (Registrant).

The scope of this compliance check decision is limited to the standard information requirement 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 after 9 March 2015, i.e. the date when the draft decision was notified to the Registrant under Article 50(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 May 2014.

On 9 March 2015 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 14 April 2015 ECHA received comments from the Registrant on the draft decision.

The ECHA Secretariat considered the Registrant's comments. The information is reflected in the Statement of Reasons (Section III) whereas no amendments to the Information Required (Section II) were made.

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

A. 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 Section 2.1.)
2) Nature and order of magnitude of any additives (Annex VI, Section 2.3.4.)
3) Description of the analytical methods (Annex VI, 2.3.7.)

B. Deadline for submitting the required information

Pursuant to Articles 41(4) and 22(2) of the REACH Regulation the Registrant shall submit the information required by this decision in the form of an updated registration to ECHA by **7 January 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 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 Section 2.1.)

ECHA concludes that the Registrant has not provided appropriate identifiers for the registered substance, as required according to Annex VI Section 2.1. of the REACH Regulation. More specifically, ECHA notes that the substance identifiers provided by the Registrant in IUCLID section 1.1 are not consistent.

The reported IUPAC name and structural information, refer to the multi-constituent substance "*reaction mass of cis-3,5-dimethyl-1,2-dioxolane-3,5-diol and trans-3,5-dimethyl-1,2-dioxolane-3,5-diol*". Such a name corresponds to a multi-constituent substance which includes the specific cyclic structure *1,2-dioxolane*. The substance described by the IUPAC name and structural information is specifically identified by EC 237-438-9 (EC name 3,5-dimethyl-1,2-dioxolane-3,5-diol) and CAS 13784-51-5.

However, ECHA notes that the Registrant identified the registered substance by EC 253-384-9 and CAS 37187-22-7 which refer to "*2,4-pentanedione, peroxide*". The identifier "*2,4-pentanedione, peroxide*" does not explicitly describe the cyclic backbone *1,2-dioxolane* and is ambiguous as it does not specify how the "peroxy" functionality is connected to the *2,4-pentanedione* structure(s). As a consequence this identifier refers to a substance which may have cyclic or non-cyclic structures.

Therefore such an identifier does not unequivocally describe the substance identified by the IUPAC name and structural formula that has been provided in the registration. Considering that substances shall be identified as precisely as possible, ECHA concludes that the Registrant did not provide appropriate information on the identification of the registered substance.

Accordingly, the Registrant is requested to clarify the identity of the substance by providing a IUPAC name which is consistent with other identifiers of the substance and ensure that the information is consistent throughout the dossier.

The Registrant is required to provide a IUPAC name and CAS entry which reflects specifically the nature of the registered substance. Furthermore, if the EC identifier currently assigned to the registered substance does not fully correspond to the registered substance, the Registrant shall not at this stage remove or modify this EC entry for technical reasons, as the registration is 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 shall refer to any available and appropriate EC number specifically corresponding to the substance.

The Registrant should note that ECHA has established processes, 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. Should the Registrant consider that the EC identifier provided in his dossier should be adapted to cover a different substance or if it actually covers several other substances, he is thus encouraged to contact ECHA for a possible adaptation of the registration.

As for the reporting of the information in IUCLID, the IUPAC name and any available CAS entry for the registered substance shall be reported in the "IUPAC name" field and under the "CAS information" header of the reference substance in IUCLID section 1.1, respectively. Should the reported CAS number not be specific but related to the registered substance, it may be reported under the "Related CAS information" header in IUCLID section 1.1. If the EC entry currently assigned does not specifically correspond to the registered substance, the Registrant shall indicate, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 253-384-9 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". The Registrant shall also specify, in the same "Remarks" field, any available and appropriate EC number for the substance (e.g. EC number 237-438-9 if the registered substance is the one identified by the IUPAC name).

The Registrant shall ensure that appropriate and consistent identifiers are used throughout the registration whenever reference to the specific substance which is the subject of this registration is made.

Further technical details on how to report the identifiers of multi-constituent substances in IUCLID are available in paragraph 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.

2) Nature and order of magnitude of any additives (Annex VI, Section 2.3.4.)

In accordance with section 2.2 of the Guidance for identification and naming of substances under REACH and CLP (version1.3, February 2014) - referred to as "the Guidance" hereinafter, an additive is a "substance that has been intentionally added to stabilise the substance". A substance being defined under Article 3(1) of the REACH Regulation by its chemical composition (i.e. "a chemical element and its compounds in the natural state or obtained by any manufacturing process..."), the role of an additive is therefore limited to preserving the integrity of the manufactured substance. In line with section 7.1 Example 'diethyl peroxydicarbonate' of the Guidance, a stabilised substance should be registered as the solution with the lowest concentration of additive which guarantees safe handling.

Intentionally added substances or solvents with other functions are not considered as additives under REACH.

ECHA notes that the Registrant indicated in IUCLID section 1.2 the additives [redacted] and [redacted] as being part of the composition of the substance. However, the information given on the additive [redacted] requires further clarification.

In the draft decision sent to the Registrant ECHA noted that the Registrant made reference to the recommended concentration level for this type of additives according to the UN Recommendations on the Transport of Dangerous Goods indicating in the remarks field of the corresponding composition block in IUCLID section 1.2 that the additives meet "*... the definition of a Type A diluent as defined in UN TDG Part 2; >= 48 % total Type A diluent...*". At the same time ECHA noted that the reported maximum concentration value ([redacted]%) for the additive [redacted] was comparatively higher than the aforementioned recommended value (>= 48 %). In addition, the reported concentration range ([redacted]%) for this additive was exceptionally broad. Therefore it was not clear if the maximum concentration level reported exceeded the concentration of additive needed to guarantee the stability of the registered substance and it was not clear if the concentration values reported were representative of the registered substance.

In the comments to the draft decision provided by the Registrant it was explained that the concentration range for the additives was reported "*...to best address all consortium member's range requirements...*". Therefore, the reason for the reported concentration range of the additive is clarified. However, the explanation indicates that the reported concentration value for the additive is not representative of the registered substance. Instead, the reported values cover all the concentration ranges of the additive of all the consortium members.

Therefore, the Registrant shall explain the reason for the need of such high concentration values of the additive [redacted] to preserve the integrity of the manufactured substance. The Registrant shall also clarify how the maximum and minimum concentration values were obtained for this additive. The reported concentration range shall not be overestimated and shall be representative of the registered substance. The Registrant shall ensure that the information is consistent throughout the dossier.

As for the reporting of the above data in the registration dossier, the information shall be included in IUCLID section 1.2

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

ECHA observes that the Registrant did not provide adequate description of the analytical methods used for the identification and quantification of the constituents required to be reported in the composition of the registered substance, as requested according to Annex VI section 2.3.7. ECHA notes that a proton nuclear magnetic resonance (^{1}HNMR) report was provided in the registration dossier, however the data submitted present some ambiguities.

More specifically, the concentration of the two main constituents (***cis**-3,5-dimethyl-1,2-dioxolane-3,5-diol* and ***trans**-3,5-dimethyl-1,2-dioxolane-3,5-diol*) was determined based on the ^{1}HNMR results, however the concentration results are not consistently reported.

The calculation of the concentration of the two isomers was based on the integration values of ^{1}HNMR signals corresponding to methyl groups. ECHA notes that in the table 6.1 (page 8) provided in the ^{1}HNMR report (*2,4-Pentanedione peroxide (CAS 37187-22-7* [redacted]), the two signals related to the methyl groups of the substances are identified with each isomer (***trans*** – signal **1a** and ***cis*** - signal **1b**). ECHA also notes that the calculated %m/m obtained based on the integration value of the signal **1a (trans)** is [redacted]**%** and on the integration of the signal **1b (cis)** is [redacted]**%** (table 6.3 of page 11 of the ^{1}HNMR report). However, in the appendix 10 (page 20) of the same report the concentration reported for the ***trans*** isomer is [redacted]**%** and for the ***cis*** isomer is [redacted]**%** (which is in agreement with the concentration values reported for the two isomers in IUCLID section 1.2).

Therefore, the Registrant shall clarify the ambiguities related to the concentration values of the two main constituents reported in the ^{1}HNMR report.

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

ECHA underlines that the compositional information reported in IUCLID Section 1.2. shall be consistent with information provided in IUCLID Section 1.4.

As for the reporting of the 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 Guilhem de Seze, Head of Unit, Evaluation E1.

[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.