EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004476-69-03/F Helsinki, 29 September 2014

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

For dipotassium peroxodisulphate, CAS No 7727-21-1 (EC No 231-781-8), 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 dipotassium peroxodisulphate, CAS No 7727-21-1 (EC No 231-781-8), submitted by [redacted] (Registrant). The scope of this compliance check 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 1000 tonnes or more per year. This decision does not take into account any updates submitted after 12 June 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 25 September 2013.

On 22 November 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 17 December 2013 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 amandments to the Information Required (Section II) were made.

On 12 June 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 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 each substance (Annex VI section 2.1 of the REACH Regulation) and molecular and structural formula (including SMILES notation) (Annex VI section 2.2.1 of the REACH Regulation).
2. 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 **5 January 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 each substance (Annex VI section 2.1 of the REACH Regulation).

"Name or other identifier of the substance" is an information requirement as laid down in Annex VI, Section 2. 1 and 2.2.1 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.

The information provided in section 1.1 of the IUCLID dossier does not allow the verification of the identity of the substance. More specifically, the EC number, EC name, CAS number, CAS name and IUPAC name provided in section 1.1 of the IUCLID dossier refer to the substance "*dipotassium peroxodisulphate*". This is also supported by the provided molecular formula and molecular weight.

However the SMILES notation, InChI code and structural formula refer to the dipotassium disulphate, which is regarded as different substance under REACH (dipotassium disulphate is covered by the EC number 232-216-8, CAS number 7790-62-7).

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit the information derived from the registered substance subject to the present decision: correct name and other identifiers, SMILES notation, InChI code and strucutral formula of the registered substance. The Registrant shall ensure that the information is consistent throughout the dossier.

In case the registered substance does not refer to the given EC number 231-781-8, then the Registrant should specify, in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 231-781-8 currently assigned does not correspond to the registered substance. This identifier can technically not be modified or deleted at this stage in the present registration update". The Registrant should also specify, in the same IUCLID field, any available and appropriate EC number for the substance.

In his comments submitted in a response to the draft decision, the Registrant indicated his intention to update the substance identifier in a way that the information provided in the registration dossier is consistent and the identity of the substance can be verified unambiguously. ECHA acknowledges the Registrant's intention to provide such information in the next update.

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

"Description of the analytical methods" is an information requirement as laid down in Annex VI, Section 2.3.7. of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

ECHA notes that the methods used by the Registrant and the description thereof for the identification of the substance are not sufficient to unambigously verify the identity of the registered substance.

The Registrant has provided the results of a fourier transform infrared (FT-IR) spectroscopy, a ultra violet (UV) spectroscopy, a mass spectroscopy (MS), a proton nuclear magnetic resonance (^{1}H-NMR) spectroscopy and semiquantitative X-ray fluorescence (XRF) spectroscopy. However these methods are not sufficient to allow an unambiguous identification of the substance as none of these methods and the results thereof provide structural information of the substance which is subject to the registration. More specifically, the MS results included in the dossier show SO_3, SO_2, SO and S fragments and the attached FT-IR spectrum shows the vibration bands associated with the S=O and S-O groups of the substance. The ^{1}H-NMR spectroscopy does not reveal any substance specific signals, as this inorganic substance does not posses hydrogen atoms in the molecule. The semiquantitative XRF analysis included in the dossier confirms the presence of potassium and sulfur in the substance, however this method cannot be used to determine the speciation of the substance. Therefore, the information provided in the registration dossier is not sufficient and does not allow ECHA to confirm the identity of the registered substance and to verify whether it refers to "*dipotassium peroxodisulphate*" or "*dipotassium disulphate*".

In his comments submitted in a response to the draft decision, the Registrant indicated his intention to update the dossier by providing additional analytical data from a titration method for the quantitative determination of the active oxygen/peroxo group content of the registered substance. ECHA acknowledges that the Registrant will update their dossier with the description of this additional titration method and with the results thereof.

However, ECHA highlights that this titration method is not specific enough to confirm unambiguously the identity of the peroxodisulfate counter ion and therefore does not provide molecular and structural information of the registered substance. In order to have a complete molecular and structural information on the registered substance, it is necessary to provide—in addition to the peroxo group titration results—analytical method and the results thereof determining the exact elemental composition of all elements present (including K, S and O) to confirm the stoichiometry of the substance.

The Registrant shall therefore provide in addition to the peroxide titration results referred to in their comments (document name: [redacted]), a description of the analytical method and the results thereof which determine the exact elemental composition (elemental ratio) of all elements present in the substance (including K, S and O).

In the draft decision, ECHA noted that for this kind of substances, ECHA expects an XRD diffractogram and relevant description to be provided. The Registrant commented that they do not see the need to provide XRD. ECHA notes that the Registrant may still provide an XRD diffractogram for the registered substance as an alternative to the above mentioned methods (titration and exact elemental composition including K, S and O contents).

Therefore, pursuant to Article 41(1) and (3) of the REACH Regulation, the Registrant is requested to submit information on an analytical method specific for the registered substance, the description of the method used and the result thereof for an unambiguous identification and quantification of the substance. ECHA underlines that in order to confirm the presence of both the potassium and peroxydisulfate ions, analytical data (description of an analytical method and the corresponding results) for the identification and quantification of each ion is required.

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/web/guest/regulations/appeals. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

[redacted]
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