ECHA
EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000004156-77-02/F Helsinki, 20 December 2013

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

For 4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane and oxydipropanol, CAS No 88288-99-7 (EC No 500-270-4), 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 dossier for 4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane and oxydipropanol, CAS No 88288-99-7 (EC No 500-270-4) 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 dossier 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 31 October 2013, 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 compliance check was initiated on 25 April 2012.

On 25 April 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. That draft decision was based on submission number [redacted].

By 27 May 2013 ECHA received comments from the Registrant agreeing to ECHA's draft decision.

On 31 October 2013 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 to amend the draft decision within 30 days of the receipt of the notification.

Subsequently, Competent Authorities of the Member States did not propose amendments to the draft decision and ECHA took the decision pursuant to Article 51(3) of the REACH Regulation.

This compliance check decision does not prevent ECHA to initiate further compliance checks on the present dossier at a later stage.

II. Information required

Pursuant to Articles 41(1), 41(3) and 10(a)(ii) as well as Annex VI , section 2 of the REACH Regulation the Registrant shall submit for the registered substance:

a. Name or other identifier of the substance (Annex VI, 2.1.);
b. Composition of the substance (Annex VI, 2.3.);
c. The description of the analytical methods or the appropriate bibliographical references for the identification of the substance (Annex VI, 2.3.7.).

Taking into consideration the data currently available in the dossier, Section III below specifies in detail all the information that ECHA considers appropriate in order to identify any substance of Unknown or Variable composition, Complex reaction products or Biological materials (UVCB). UVCB substances cannot be sufficiently identified by their chemical composition, because the number of constituents is relatively large; and/or the composition is, to a significant part, unknown; and/or the variability of composition is relatively large or poorly predictable. As a consequence, UVCB substances require other types of information for their identification, in addition to what is known about their chemical composition.

As a result, ECHA cannot be in a position, before receiving suitable information, to determine precisely the other types of information that is actually required to identify a specific UVCB substance. Only the Registrant of that UVCB substance knows the details of its identity. Based on this knowledge, he may consider that some of the information requested by ECHA is not suitable and necessary in order to identify the substance. Nevertheless, it is the Registrant's exclusive responsibility 1) to ensure that ECHA is in a position to identify precisely the substance and 2) to justify the reasons for which some information requested may have been omitted.

Therefore, if the Registrant eventually decides to submit only part of the detailed information specified in Section III and if the submitted information does not enable ECHA to establish and verify the identity of the substance actually covered by the dossier, the registration will not be considered valid.

Pursuant to Article 41(4) of the REACH Regulation the Registrant shall submit the information in the form of an updated IUCLID dossier to ECHA by **20 March 2014**.

III. Statement of reasons

Based on the examination of the technical dossier, ECHA concludes that the information therein, submitted by the Registrant for registration of the above mentioned substance for the purpose of registration within the applicable tonnage band of 1000 tonnes or more per year in accordance with Article 6 of the REACH Regulation, does not comply with the requirements of Articles 10 and with Annex VI thereof. Consequently, the Registrant is requested to submit the information mentioned above that is needed to bring the registration into compliance with the relevant information requirements.

Pursuant to Article 10(a)(ii) and Annex VI, section 2 of the REACH Regulation, the technical dossier of the registration shall include information on the identity of the substance. Annex VI, section 2 lists information requirements that shall be sufficient to identify the registered substance.

(a) Name or other identifier of the substance (Annex VI, 2.1. of the REACH Regulation)

ECHA notes that the Registrant identified the registered substance as a substance 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 shall consist of two parts: (i) the chemical name and (ii) a more detailed description of the manufacturing process, as described 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 explained under points (i) and (ii) thereinafter).

(i) Information on the chemical name to be submitted by the registrant

The IUPAC name provided for the registered substance (propane-1,2-diol polymer with 1-isocyanato-4-[(4-isocyanatophenyl)methyl]benzene and 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene) specifies that propane-1,2-diol (EC 200-338-0) is used as starting material.

At the same time ECHA notes that the Registrant assigned to the registered UVCB substance the EC number 500-270-4 (EC name: 4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane and oxydipropanol) and CAS number 88288-99-7 (CAS name: Propanol, oxybis-, polymer with 1-isocyanato-2-[(4-isocyanatophenyl)methyl]benzene and 1,1'-methylenebis[4-isocyanatobenzene]). Based on these identifiers this UVCB substance is obtained from the starting materials 4,4'-Methylenediphenyl diisocyanate, 2,4'-diisocyanatodiphenylmethane and oxydipropanol.

ECHA notes that the starting material propane-1,2-diol specified in the IUPAC name is not mentioned in the EC and CAS entries. ECHA concludes that the substances described by the EC and CAS identifiers do not correspond to the substance described by the IUPAC name.

Furthermore the EC and CAS names provided for the registered substance specify oxydipropanol (CAS: Propanol, oxybis-) as starting material. The Registrant shall note that the generic name "oxydipropanol" corresponds to a multi-constituent substance including all possible isomers of oxydipropanol. ECHA notes, that the structural formula given in section 1.1 of the IUCLID dossier for the registered substance and in section 1.2 for the group of constituents "higher oligomers" indicates that only 1,1'-oxydipropan-2-ol is used as starting material.

As a consequence, the information included in the EC and CAS identifiers in relation to the starting materials is not consistent with the information that can be derived from the structural formula given in section 1.1 and 1.2 of the registration dossier.

In addition the generic term "polymer" is included in the CAS and IUPAC name, whereas the EC name refers more specifically to the manufacturing of an oligomeric substance. The Registrant shall note that the IUPAC name shall specifically correspond to the substance that is registered.

ECHA notes also that the EC entry 500-270-4 specified for the registered substance is included in the No-Longer Polymer (NLP) list (available on esis.jrc.ec.europa.eu website). In such list, the EC entry 500-270-4 is actually linked to CAS entry 88288-99-7. The Registrant shall note, however, that as explained in the NLP list (page 8 of the document) "*NLP-Nos and name descriptions take precedence. The CAS-RN given are to be treated as indicative*

and for a use as a searching tool". ECHA considers that the CAS information included in the registration dossier is generic and does not fully correspond to the registered substance.

Accordingly, the Registrant is required to provide the chemical name which reflects the oligomeric nature of the registered substance and includes the specific IUPAC name (or the specific chemical name derived according to the Guidance) of the starting materials used. As for the reporting of the information in IUCLID, the IUPAC name and any available CAS entry for the registered substance should be reported in the "IUPAC name" field and under the "CAS information" header of the reference substance in IUCLID section 1.1, respectively. The CAS entry with CAS number 88288-99-7 may be reported under the "Related CAS information" header in IUCLID section 1.1.

In case when the EC and CAS identifiers do not fully correspond to the registered substance (e.g. the identity of the starting materials requested under point (ii) do not correspond to the substance named oxydipropanol), the Registrant shall ensure to delete the CAS information and indicate in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The EC entry 500-270-4 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 should also specify, in the same "Remarks" field, any available and appropriate EC number for the substance.

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.

(ii) A detailed manufacturing process description to be submitted by the registrant

Based on the information provided by the Registrant regarding the composition of the registered substance, ECHA concludes that the exact identity and concentration levels of the individual constituents reported in section 1.2 of the updated dossier are not sufficiently known for the UVCB substance to be identified by its composition alone. ECHA also underlines that the chemical name used by the Registrant to identify the registered substance, which is based on its starting materials, does not allow for an accurate and complete identification of the substance. A detailed description of the manufacturing process, including the chemical identity of the starting materials and information on the most relevant steps of the manufacturing process, is therefore required.

1) <u>The identity of the starting materials used (in terms of identity and upper and lower concentration levels of each individual constituent) must be submitted</u>

The Registrant identified generically the starting materials used for the manufacturing of the registered substance as MDIs (EC 500-079-6 or 905-806-4 or 247-714-0 or 202-966-0 or 227-534-9) or hydroxy or amino compounds. The identity of the starting materials has not been specified to a sufficient level of detail as the description does not include any information on the exact identity and predominance of the individual constituents which the starting materials consist of. ECHA considers that the composition of the starting materials is one of the factors determining the composition of the registered substance. Information on the name and composition of those starting materials (in terms of identity and upper and lower concentration levels of each individual constituent) is therefore necessary for the identification of the registered substance.

The Registrant is accordingly required to provide the specific IUPAC name (or the specific chemical name derived according to the Guidance) and EC and CAS identifiers of every single starting material as well as the identity and upper and lower concentration level of each constituent present in the composition of the starting materials. The Registrant shall ensure that the specific starting materials generically designated as MDIs (EC 500-079-6 or 905-806-4 or 247-714-0 or 202-966-0 or 227-534-9) or hydroxy or amino compounds in the registration dossier is designated using a chemical name that accurately reflects their identity. Further information for the identification and naming of substances, including the starting materials, is available in the Guidance.

2) The description of the manufacturing processing steps must be submitted by the registrant

ECHA observes that the description of the manufacturing process is not sufficiently detailed for the identification of the registered substance. More specifically, the Registrant states generically that the registered substance is "prepared from MDIs (EC 500-079-6 or 905-806-4 or 247-714-0 or 202-966-0 or 227-534-9) via potentially catalyzed partial reaction with themselves or with hydroxy or amino compounds resulting in molecules terminated with isocyanate groups." However, no further information has been specified on the manufacturing process parameters which can determine the composition of the registered substance and therefore its identity.

The Registrant is accordingly required to provide details of the manufacturing processing steps that are applied to the starting materials, in the order they occur. The information submitted by the Registrant must at least include the following:

- Ratio of all starting materials shall be specified.
- Description of the manufacturing steps in the order they occur. Each step, including preliminary steps, steps involving chemical transformation, isolation and purification steps shall be specified.
- For each step, all relevant process parameters that affect the composition and therefore the identity of the substance must be provided.
- Description of the reactions occurring during each step leading to the formation of unintended constituents shall be provided.
- Regarding more specifically the steps involving a chemical transformation, the Registrant shall describe of the oligomerisation, including the parameters used to initiate, propagate and terminate the oligomerisation reactions. The information shall be supplemented with details of the reaction mechanisms involved. Where the oligomerisation involves catalytic reactions, the information shall include, for each catalytic reaction, details of the type of catalyst(s) used in terms of reaction(s) that they catalyse (including detailed information on the selectivity of the catalyst towards the reaction products, reaction mechanisms etc.). The information on how the use of the specific catalyst affects the composition of the registered substance must be also included. The present request is not limited to the catalytic reactions, but concerns all oligomerisation steps.

If the substance covered by the registration is manufactured according to different manufacturing processes, including the use of different sources, then the detailed description of the manufacturing process required under points (ii) 1) and (ii) 2) hereinabove shall be reported separately for each manufacturing process. A manufacturing

process may be considered different when the processing steps and/or processing parameters are different.

The Registrant shall note that substances manufactured according to different manufacturing processes may indicate multiple substances and consequently the requirement for multiple registrations.

Regarding how to report the description of the manufacturing process of the UVCB substance, the information shall be included in the Description field in IUCLID section 1.1.

b) Composition of the substance (Annex VI, 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 corner stone of all the REACH obligations.

ECHA notes that the registration does not contain sufficient information for establishing the composition of the registered substance and therefore its identity, as required under Annex VI, section 2.3. of the REACH Regulation.

More specifically, the Registrant indicated overly broad concentration ranges for the constituents reported in the IUCLID dossier. In particular, the concentration range for 4,4'-methylenediphenyl diisocyanate, for o-(p-isocyanatobenzyl)phenyl isocyanate and for "higher oligomers of MDI/DPG" vary from [redacted] to [redacted] % (w/w), from [redacted] to [redacted] %(w/w) and from [redacted] to [redacted] %(w/w) respectively.

Such wide concentration ranges are not justified by the manufacturing process description due to its lack of detail (see section III.a above).

Furthermore the Registrant shall note that in line with the Guidance, substances in which one constituent is present at a concentration >80% (w/w) are regarded as mono-constituent substances. As a consequence a substance including [redacted]% of 4,4'-methylenediphenyl diisocyanate would normally be regarded as the mono-constituent substance "4,4'-methylenediphenyl diisocyanate". Such substance is regarded as a different substance from "4,4'-Methylenediphenyl diisocyanate, oligomeric reaction products with 2,4'-diisocyanatodiphenylmethane and oxydipropanol" for which separate registration obligations apply under REACH.

In addition, ECHA observes that the specific identity and concentrations of the constituents which the "higher oligomers of MDI/DPG" consist of have not been provided.

Therefore ECHA concludes that the information provided on the composition is not sufficient to have a chemical representation of what the substance consists of.

According to chapter 4.3 of the Guidance on substance identification, for UVCB substances such as the registered substance, the Registrant shall provide the following:

- 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 identified and reported individually; and

- Unknown constituents shall be identified as far as possible by a generic description of their chemical nature. The identification of these other constituents must be provided in order to allow ECHA to establish the composition of the substance as manufactured and to use the compositional information as one identifier for the registered substance. This information must also allow ECHA to verify that the composition is consistent with the chemical name reported for the registered substance. Regarding the reporting of the constituents identified as "higher oligomers of MDI/DPG" a distinction according to the degree of oligomerisation and to the type of termination is required for this purpose as a baseline.

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

In line with the above, the Registrant is requested to revise the concentration ranges provided for the constituents specified in section 1.2 of the IUCLID dossier and to include specific information on the identity and concentration of the different groups of oligomers present in the substance.

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, shall be reported in the appropriate fields in IUCLID. For the unknown 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.

The concentration range values must be representative for the registered substance as manufactured and it shall be clarified how the minimum and maximum concentration values for each group of constituents were obtained (i.e. information on the batch selection, sampling procedure, the measured values, calculations used etc.). Without this information ECHA is not able to conclude on the representativeness of these values and the identity of the substance covered by the registration shall not be considered valid.

Where the Registrant covers different grades of the same substance in a registration, the Registrant shall report separately the compositional information of each grade.
This means that if the substance covered by the registration has two (or more) different compositions, then these must be presented separately. Information on how to report several compositions in IUCLID is specified in paragraph 2.3, Q&A8 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), available on the ECHA website.

ECHA highlights that failure to report separately the compositional information of each grade of a substance may result in one or more grades not being covered by this registration.

The Registrant should also note that multiple compositions may indicate multiple substances and consequently the requirement for multiple registrations.

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).

The Registrant shall ensure that the information provided on the composition of the substance is confirmed by the analytical data included in section 1.4 of the IUCLID dossier.

c) Description of the analytical methods (Annex VI, section 2.3.7 of the REACH Regulation)

ECHA observes that the Registrant did not provide sufficient description of the analytical method used for the identification and quantification of the different constituents present in the composition of the registered substance, which is required according to Annex VI section 2.3.7.

More specifically ECHA notes the following incompliances:

- The Registrant provided an analytical report of a Gel Permeation Chromatography showing the presence of "higher oligomers" in the substance. Such information, however, does not provide any information on the identity and concentration of the specific oligomers present in the substance.
- The Registrant did not provide an explanation on how the analytical results translate to the composition specified in section 1.2 of the registration dossier. The Registrant provided an insufficient description of the chromatographic method used for the quantification of the constituents shown in the chromatogram. Information on how the peaks have been allocated, standard used and how the %Area values shown in the chromatogram have been converted into the concentration values reported in section 1.2 of the IUCLID dossier have not been provided.

The Registrant is accordingly requested to select analytical methods enabling the identification and quantification of the constituents and groups of constituents required to be reported in the composition of the registered substance and quoted under point III b) of this decision and to provide the description of these analytical methods. 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. If the description is not sufficient for the method to be reproduced by any third party laboratory, ECHA will consider the description insufficiently detailed. In that case, the information requirement under Annex VI section 2.3.7 will not be fulfilled.

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

The composition reported in the dossier must be fully consistent with the analytical results obtained.

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.

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