~~CONFIDENTIAL~~

European Chemicals Agency

Decision number: CCH-D-0000001638-68-03/F Helsinki, 1 August 2011

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

For Isododecane (CAS No. 93685-81-5, EC No. 297-629-8), 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 dossier for **isododecane (CAS No. 93685-81-5, EC No. 297-629-8)** submitted by [redacted] (Registrant), latest submission number [redacted], for ≥ 1000 tonnes per year.

The compliance check was initiated on 31 March 2011.

On 27 April 2011 ECHA notified the Registrant of its draft decision and invited him pursuant to Article 50(1) of the REACH Regulation to provide comments within 30 days of the receipt of the draft decision.

On 27 May 2011 the Registrant provided to ECHA comments on the draft decision. ECHA reviewed the further information received and amended the draft decision by extending the deadline to submit an updated IUCLID dossier to 4 months from the date of the decision.

On 17 June 2011 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. 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

1) Pursuant to Articles 41(1)(a), 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. The composition (Annex VI, 2.3): any information which is suitable and necessary to allow ECHA to establish and verify the composition and the name of the registered substance, as specified under section III.1.a. below;
b. The spectral data (Annex VI, 2.3.5): an infra-red spectrum;
c. The description of the analytical methods (Annex VI, 2.3.7): a description of the analytical methods, or the appropriate bibliographical references, to identify the registered substance, including its composition. The information shall be sufficient for each method to be reproduced and shall therefore include details of the experimental protocol followed, the calculation used and the result obtained.

2) Pursuant to Articles 41(1)(a) and (b), 41(3), 10(a)(vi) and (ix), 12(1)(e), 13 and Annexes X and XI of the REACH Regulation, the Registrant shall submit information on:

a. The identity of the substance intended to be tested in the proposed two-generation reproductive toxicity study, as specified under section III.2 below. In particular, the information to be provided shall include the chemical name or any other equivalent identifier of the substance to be tested and its specific composition as described under point 1(a) for the registered substance.

3) Pursuant to Articles 41(1)(a) and (b), 41(3), 10(a)(vi) and (ix), 12(1)(e), 13 and Annexes X and XI of the REACH Regulation, the Registrant shall submit:

a. If the substance specified in point 2 above is not the registered substance, a justification detailing and documenting why it would fulfil the information requirement of Annex X, section 8.7.3 for the registered substance, as specified under section III.3 below.

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 **2 December 2011 - 4 months from the date of the decision**.

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 in accordance with Article 6 of the REACH Regulation, does not comply with the requirements of Articles 10, 12 and 13 and with Annexes VI, X and XI 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.

1) Missing information related to substance identity

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) Composition of the registered substance (Annex VI, 2.3)

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 information, sufficient for establishing the composition of the registered substance and therefore its identity, which is required under Annex VI, Section 2.3 of the REACH Regulation. More specifically, ECHA notes that the Registrant does not provide any information on the identity and concentration of the different constituents or groups of constituents which the substance consist of. While the analytical information provided in section 1.4 of IUCLID indicates that the analysed substance consists of hydrocarbons from C8 to C16 (with a predominance of 2,2,4,6,6-pentamethylheptane), the Registrant does not report, in section 1.2 of IUCLID, the presence of any of the constituents and their typical concentrations and concentration ranges. Therefore, the substance identity, including the chemical name, could not be verified.

Following section 4.3 of the Guidance for identification and naming of substances under REACH[1], the Registrant should note that for UVCB substances (substances of Unknown or Variable Composition, or of Biological origin) presenting a large number of constituents, 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 constituents relevant for the classification and/or PBT assessment of the registered substance shall be identified and reported individually; and

- Other constituents shall be identified 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. The Registrant must provide any information which is suitable and necessary to meet these objectives.

  For UVCB substances, such as the registered substance, the reporting of such other constituents according to the hydrocarbon classes to which they belong is necessary for this purpose. The hydrocarbon classes to be reported should include any hydrocarbon class present in the composition of the registered substance (such as branched alkanes, linear alkanes, cycloalkanes, as appropriate) independent of their concentration. For each hydrocarbon class, the carbon number range should at least be reported in order to set the limits of the constituents covered.

In line with the above, the Registrant is requested to provide any information which is suitable and necessary to allow ECHA to establish and verify the composition and the name of the registered substance. 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.

Regarding how to report the composition of the registered substance in IUCLID, the following applies: the Registrant shall report the composition of the registered substance in IUCLID section 1.2. For each constituent required to be reported individually, the IUPAC

[1] http://guidance.echa.europa.eu/docs/guidance_document/substance_id_en.pdf

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 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), the carbon number range, as well as the minimum, maximum and typical concentration, shall be reported in the appropriate fields in IUCLID.

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 18 on the ECHA website[2].

(b) The spectral data (Annex VI, 2.3.5): infra-red spectrum

ECHA points out that the registration does not contain any infra-red spectral data which is required according to Annex VI, Section 2.3.5 of the REACH Regulation to support the indicated substance identity. Instead, the Registrant includes justifications for not providing this information. According to the justifications, the Registrant considers that "no value is added" by the required spectral data.

ECHA, however, points out that the infra-red spectral data is a standard requirement of Annex VI, Section 2.3.5. Contrary to the Registrant's justifications, ECHA regards the required infra-red spectral data as scientifically necessary for the identification of the registered substance because the infra-red spectrum displays characteristic vibration bands of the molecules present in the substance. Although no functional groups might be present in the molecules indicated in the chemical name, alkanes such as isoalkanes have characteristic vibration bands which should be recorded in the spectrum. As a consequence, the infra-red spectrum provides information on the identity of the substance.

Therefore, the Registrant is requested to submit an infra-red (IR) spectrum.

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

(c) The description of the analytical methods or the appropriate bibliographical references for the identification of the substance (Annex VI, 2.3.7)

ECHA observes that the Registrant provides a description of a gas chromatographic analytical method used for the identification and quantification of hydrocarbons. The Registrant reports the result of the analysis by specifying the concentration of groups of hydrocarbons according to their carbon numbers. However ECHA notes that the description of the method does not include any qualitative and quantitative information on the individual constituents present in the registered substance. ECHA points out that the quantitative ^{13}C-NMR spectral analysis attached in the dossier indicates the clear predominance of one specific constituent (2,2,4,6,6-pentamethylheptane) which has not been quantified as such. As a result of these observations, ECHA can not verify that all constituents required to be reported individually have been identified and quantified.

[2] http://echa.europa.eu/doc/reachit/dsm18/substance_id_report_iuclid_en.pdf

Accordingly, in line with Annex VI, 2.3.7, the Registrant is requested to submit the description of the missing analytical methods, or the appropriate bibliographical references, used to identify the registered substance, including its composition. The information shall be sufficient for each method to be reproduced and shall therefore include details of the experimental protocol followed, the calculation used and the results obtained.

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

2) Missing information related to the endpoint concerned

ECHA notes that the Registrant intends to cover the information requirement for a two-generation reproductive toxicity study (a standard requirement of Annex X, 8.7.3) by performing a test according to OECD guideline 416. The Registrant proposes to perform this test with a substance to be selected from a hydrocarbon solvent group of UVCB substances. The Registrant does not specify the identity and composition of this substance.

If the Registrant suggests carrying out the proposed test required by Annex X on another substance than the registered substance, Article 13(1) and Annex X, third introductory paragraph, of the REACH Regulation require the Registrant to clearly state reasons for adapting the standard information according to the rules in Annex XI. This includes that similarity between the registered substance and the substance to be tested needs to be established by the Registrant.

ECHA concludes that as the identity and composition of the substance to be tested was not provided in the registration dossier, the similarity between the substance to be tested and the registered substance could not be considered, and that therefore the requirements of Annex XI, section 1.5, as explained below, in conjunction with Article 13(1) and Annex X, third introductory paragraph, of the REACH Regulation are not met.

The Registrant is accordingly requested to submit the information concerning the identity and composition of the substance to be tested. The information to be provided shall include the chemical name or any other equivalent identifier of the substance to be tested and its specific composition as described under point 1(a) for the registered substance.

Regarding how to report the identity of the test substance in IUCLID, the following applies: the Registrant should report the name or any other equivalent identifier of the substance in the "test material identity" field of the endpoint study record. The constituents or group of constituents required to be specified shall be identified by a chemical name. The concentration of these constituents in the substance to be tested shall also be reported. The information on the composition shall be reported in either the "details on test material" or "confidential details on test material" field of the endpoint study record.

3) Missing information concerning the use of read across / grouping approach

The technical dossier submitted by the Registrant contains a general statement for the use of a grouping approach including four categories and a category justification document for "Category 8: C9–C14 Aliphatics (< 2 % aromatics)"[3] to which the registered substance

[3] Assumed Category 8; the CSR attached to the Registration dossier contains inconsistent numbering of the categories.

reportedly belongs. The substance to be tested is reported to be selected from another category, namely "Category 3: C9–C14 Aliphatics (2–25 % aromatics)". No comparison between the registered substance and the substance to be tested was included in the registration dossier. Furthermore, no comparison between the categories of these two substances was provided to further justify the read-across between the two substances. If the Registrant proposes to carry out the proposed test on another substance than the registered substance, it is thus not clear from the registration dossier on which grounds listed in Annex XI, section 1.5 governing grouping of substances and read-across this grouping approach is based on.

Article 13(1) and Annex X, third introductory paragraph, of the REACH Regulation require the Registrant to clearly state reasons for adapting the standard information according to the rules in Annex XI. More specifically, Annex XI, section 1.5 provides that substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity may be considered as a group, or 'category' of substances. Application of the group concept requires that physicochemical properties, human health effects and environmental effects or environmental fate may be predicted from data for reference substance(s) by interpolation to other substances in the group (read-across approach).

The similarities may, according to Annex XI, section 1.5, be based on:

(1) common functional group;
(2) the common precursors and/or the likelihood of common breakdown products via physical or biological processes, which result in structurally similar chemicals; or
(3) a constant pattern in the changing of the potency of the properties across the category.

In addition, in order to justify the group concept according to Annex XI, section 1.5, it should be clear for which endpoints the suggested read-across is applicable. Annex XI, section 1.5 requires that the results (i) are adequate for the purpose of classification and labelling and/or risk assessment, (ii) have adequate coverage of the key parameters and cover an exposure duration addressed in the corresponding test method referred to in Article 13(3) and (iii) that the documentation of the applied method is adequate and reliable.

ECHA points out that the category justification presented in the registration dossier does not specify for each of the substances to be included in the category of the registered substance and the constituents of these substances, which information on the physicochemical properties, human health effects and environmental effects is available. Moreover, the registration dossier does not provide such information concerning the substance to be tested or the category of the substance to be tested.

Furthermore, the information provided in IUCLID section 7.8.1 and the documents attached in IUCLID section 13 of the dossier provides inconsistent lists with regard to how many and which substances are members of the category of the registered substance.

The similarity of substances, as required under Annex XI, section 1.5, needed for a group or category of substances could not be considered. Therefore the requirements of Annex XI, section 1.5 in conjunction with Article 13(1) and Annex X, third introductory paragraph, of the REACH Regulation are not met.

Taking into account the substance identity information requested under point 1 and the identity of the substance to be tested requested under point 2, the Registrant is thus

requested to submit a justification detailing why the proposed test on the substance specified in point 2 above would fulfil the information requirement of Annex X, section 8.7.3 for the registered substance in line with Annex XI, section 1.5. This applies if the substance specified in point 2 above is not the registered substance.

In order to further justify the above-mentioned read-across, further information on the grouping approach must also include the identity of the substances that are members of the categories of the registered substance and the substance to be tested, their constituents and clear indication for which substances or their constituents test data on the physicochemical properties, human health effects and environmental effects exist as well as information on the production processes that could further justify the grouping approach. This issue is further reported in paragraphs 6.2.5 and 6.2.6 of the Guidance on QSARs and grouping of chemicals[4]. This above-mentioned information on physicochemical properties, human health effects and environmental effects that are used to justify the grouping approach should also be reported in the IUCLID registration dossier in a form of robust study summaries or study summaries.

4) Timeline to submit an updated IUCLID dossier

On 27 April 2011 the Registrant was notified of the draft decision and was invited to comment within 30 days. In his comments on 27 May 2011 the Registrant proposed to extend the submission deadline of an updated IUCLID dossier from 2 months to 6 months of the date of the decision. ECHA evaluated the justification for this extension and acknowledges that the needs to coordinate the actions between the Registrants of the category and the other justifications given justify extending the deadline by 2 months. Nevertheless the issues addressed in this decision do not involve performance of long-term studies which would necessitate a further extension of the deadline. Therefore ECHA decided to extend the deadline from 2 months to 4 months from the date of the decision.

IV. General requirements for the generation of information and Good Laboratory Practice

ECHA always reminds registrants of the requirements of Article 13(4) of the REACH Regulation that reads:

> "Ecotoxicological and toxicological tests and analyses shall be carried out in compliance with the principles of good laboratory practice provided for in Directive 2004/10/EC or other international standards recognised as being equivalent by the Commission or the Agency and with the provisions of Directive 86/609/EEC, if applicable."

According to Article 13(3) of the REACH Regulation, tests that are required to generate information on intrinsic properties of substances shall be conducted in accordance with the test methods laid down in a Commission Regulation or in accordance with other international test methods recognised by the Commission or the European Chemicals Agency as being appropriate. Thus, the Registrant shall refer to Commission Regulation (EC) No 440/2008 laying down test methods pursuant to Regulation (EC) No 1907/2006 as adapted to technical progress and use the applicable test methods to generate the information on the endpoints indicated above.

[4] http://guidance.echa.europa.eu/docs/guidance_document/information_requirements_r6_en.pdf?vers=20_08_08

National authorities monitoring good laboratory practice (GLP) maintain lists of test facilities indicating the relevant areas of expertise of each facility.

V. 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 website[5]. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

Done at Helsinki,

Geert Dancet
Executive Director

[5] http://echa.europa.eu/appeals/app_procedure_en.asp