~~CONFIDENTIAL~~

European Chemicals Agency

Decision number: CCH-D-0000001633-78-03/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 tetradecane (CAS 629-59-4, EC No. 211-096-0), 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 the ECHA has performed a compliance check of the registration dossier for **tetradecane (CAS 629-59-4, EC No. 211-096-0)** submitted by [redacted] (Registrant), latest submission number [redacted], for over 1000 tonnes per year.

The compliance check was initiated on 24 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): Information on the identification and quantification of the impurities and, as specified under section III.1.a. below;

b. The spectral data (Annex VI, 2.3.5): infra-red (IR) spectrum and nuclear magnetic resonance (NMR; such as ^{1}H-NMR) spectrum. As an alternative to the NMR spectrum, a mass spectroscopic analysis of the registered substance can be provided;
c. A high-pressure liquid chromatogram or gas chromatogram (Annex VI, 2.3.6), as specified under section III.1.c. below; and
d. The description of the analytical methods (Annex VI, 2.3.7): 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 results 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 point III.2 below.

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 point 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, which is required under Annex VI, Section 2.3 of the REACH Regulation.

More specifically, ECHA observes that the registered substance is a mono-constituent substance. ECHA points out that because mono-constituent substances are, by definition, composed of only one main constituent, the minimum concentration of that constituent in the registered substance (i.e. [redacted], as specified in the dossier) indicates that the total amount of impurities reaches up to [redacted]. The Registrant has not reported the presence of any impurity in the composition of the substance. Therefore [redacted]% of the composition of the substance is not accounted for. ECHA can thus not verify that all individual impurities required to be identified have been reported in the composition of the registered substance.

In line with paragraph 4.2 of the Guidance for identification and naming of substances under REACH[1], the following applies to all mono-constituent substances, including the registered substance:

- All the impurities present at ≥ 1 % are required to be reported; and
- All constituents relevant for the classification and/or PBT assessment of the registered substance shall be reported.

The Registrant is accordingly requested to complete or correct the above information on the composition of the registered substance provided in the registration dossier, in order to allow ECHA to have a precise chemical representation of what the substance consists of. 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 individually any impurity required to be identified and specify least one of the following identifiers: chemical name, CAS number, EC number and/or molecular formula, as well as the minimum, maximum and typical concentration, in the appropriate fields in Section 1.2 of the IUCLID dossier. The Registrant shall also provide accurate information on the degree of purity of the registered substance and/or the concentration range of the main constituent and any impurity reported in Section 1.2 of the IUCLID dossier to ensure that the information provided is consistent.

Further technical details on how to report the composition of mono-constituent substances in IUCLID are available in paragraphs 2.1 and 2.2.1.1 of the Data Submission Manual 18 on the ECHA website[2].

(b) The spectral data (Annex VI, 2.3.5)

ECHA points out that the registration contains neither IR nor NMR spectral data which are 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 provided, the Registrant considers the required spectral data as scientifically unnecessary to identify the substance.

[1] http://guidance.echa.europa.eu/docs/guidance_document/substance_id_en.pdf
[2] http://echa.europa.eu/doc/reachit/dsm18/substance_id_report_iuclid_en.pdf

ECHA, however, points out that spectral data is a standard requirement of Annex VI, Section 2.3.5. Contrary to the Registrant's justifications, ECHA regards the required spectral data as scientifically necessary for the identification of the registered substance for the following reasons:

- The IR spectrum displays characteristic vibration bands of the molecules present in the substance. Although no functional groups might be present in the molecule indicated in the chemical name, alkanes have characteristic vibration bands which should be recorded in the spectrum. As a consequence, the IR spectrum provides information to verify the identity of the substance; and
- An NMR spectrum, such as ^{1}H-NMR, is a relevant tool for molecular structure characterization of well-defined organic substances due to characteristic chemical shifts and spin-spin coupling, which also reflect the relative abundance of individual atoms.

Therefore, the Registrant is requested to submit an IR spectrum and an NMR spectrum, such as a ^{1}H-NMR. As an alternative to the NMR spectrum, a mass spectroscopic analysis of the registered substance can be provided.

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

(c) A high-pressure liquid chromatogram or gas chromatogram (Annex VI, 2.3.6)

ECHA notes that the registration does not include any high-pressure liquid chromatogram or gas chromatogram, which is required according to Annex VI, Section 2.3.6 of the REACH Regulation. ECHA observes that the Registrant refers to a gas chromatogram in the IUCLID dossier. However, the Registrant did not attach such report in the dossier. ECHA points out that the chromatographic analysis of organic substances such as the registered substance enables the separation and individual detection of the constituents present in the substance. ECHA therefore regards the required chromatogram as scientifically necessary to support the indicated substance identity.

Accordingly, the Registrant is requested to submit a high-pressure liquid chromatogram or gas chromatogram. The Registrant shall ensure that the information provided does not only include the copy of the chromatogram but also the report of the peak list with the associated retention times and peak area. The peak list and the associated retention times and peak area is required since this information constitutes a numerical representation of the chromatogram.

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

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

ECHA observes that the registration does not contain any description of the qualitative and quantitative analytical methods used to identify the registered substance, including its composition, as required by Annex VI, Section 2.3.7 of the REACH Regulation.

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, 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 of 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 an UVCB substance to be selected from a hydrocarbon solvent group of 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, 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 of the substance to be tested and the registered substance could not to be considered, and 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.

When clarifying the identity of the substance to be tested, the Registrant should note that, if the substance to be tested is an UVCB substance from a hydrocarbon solvent group, it is required to be identified by the chemical name or any other equivalent identifier of the substance and its specific composition. Concerning the reporting of the composition of such UVCB 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 test substance to be selected from the group, 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 not only the hydrocarbon classes referred to in the chemical name of the substance (i.e. linear alkanes, branched alkanes, cycloalkanes and aromatic hydrocarbons) but also any other hydrocarbon class present in the composition of the substance to be tested (such as linear alkenes, branched alkenes, cycloalkenes and any other hydrocarbon class, as appropriate). For each hydrocarbon class, the carbon number range should at least be reported in order to set the limits of the constituents covered. Information on the number of aromatic rings in the constituents covered under the aromatic hydrocarbon class should also be provided to further set the limits of the constituents covered under that specific entry.

In line with the above, the Registrant must provide any information which is suitable and necessary to allow ECHA to establish the identity of the substance to be tested.

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 should 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 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, require 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 approach 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] However, the CSR attached to the registration dossier contains inconsistent numbering of the categories.

(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 under IUCLID section 7.8.1 and the documents attached in IUCLID section 13 of the dossier provided 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 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

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

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 the technical progress, and use the applicable test methods to generate the information on the endpoints indicated above.

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,

[redacted]

Geert Dancet
Executive Director

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