EUROPEAN CHEMICALS AGENCY

Decision number: CCH-D-0000002301-90-03/F Helsinki, 24 April 2012

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

For Vinyl neononanoate, CAS No 54423-67-5 (EC No 259-160-7), 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 Vinyl neononanoate, CAS No 54423-67-5 (EC No 259-160-7) submitted by [redacted] (Registrant), with submission number [redacted], for 100 - 1000 tonnes per year.

The compliance check was initiated on 12 August 2010.

On 28 March 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 21 April 2011 the Registrant provided to ECHA comments on the draft decision. On 18 May 2011 the Registrant submitted an updated IUCLID file to ECHA [redacted] the registration tonnage at 100-1000 tonnes per year. Two testing proposals were included in the updated dossier.

ECHA reviewed the further information received and amended the draft decision accordingly, targeted to the information requirements of Annex VIII of the REACH Regulation.

On 21 January 2012 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.

The present decision relates solely to the compliance check process. The outcome of the testing proposals examination will be addressed in a separate decision.

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) Spectral data: ultra-violet and nuclear magnetic resonance and/or mass spectra (Annex VI, 2.3.5.);
   b) Chromatographic data that enables the composition to be quantified (Annex VI, 2.3.6). This shall include a description of how the composition of the substance was quantified based on the chromatographic data;
   c) The description of the analytical methods or the appropriate bibliographical references for the identification of the substance and the additive. This information shall be sufficient to allow the method to be reproduced (Annex VI, 2.3.7.).

2) Pursuant to Articles 41(1)(a), 41(3) 10(a)(vi) and (vii), as well as Annex VII and VIII of the REACH Regulation the Registrant shall submit the following information using the test method indicated below:

   - Boiling point (Annex VII, 7.3.; EU Method A.2);
   - Vapour pressure (Annex VII, 7.5.; EU Method A.4);
   - Auto-ignition temperature (Annex VII, 7.12.; EU Method A.15).

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 **24 April 2013**.

At any time, the Registrant shall take into account that there may be an obligation to make every effort to agree on sharing of information and costs with other registrants.

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 [redacted] in accordance with Articles 6 and 11(2) of the REACH Regulation, does not comply with the requirements of Articles 10, 12 and 13 and with Annexes VII and VIII thereof. During the course of this compliance check, the Registrant updated his dossier to a tonnage band of 100-1000 tonnes per year. This compliance check is targeted to compliance with the requirements of Articles 10, 12 and 13 and with Annexes VII and VIII 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.
In his comments, the Registrant expressed consent to submit the missing information that is subject to the present decision.

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. The technical dossier contains only an infra-red spectrum of the substance, which alone is not sufficient to verify the substance identity. The technical dossier does not contain ultra-violet, nuclear magnetic resonance, or mass spectra, and does not contain a justification for omitting these spectra. These are required under Annex VI, 2.3.5. The Registrant shall therefore provide an ultra-violet spectrum in addition to a nuclear magnetic resonance and/or mass spectrum for the registered substance.
b. The technical dossier contains a gel permeation chromatogram that does not enable the substance composition to be quantified. The Registrant is obliged by Annex VI, 2.3.6 to submit chromatographic data that enables the composition to be quantified. The Registrant is required to include a description of how the composition was quantified based on the chromatographic data.
c. The registration did not contain details of analytical methods to determine the main constituent and the additive which is required by Annex VI, Section 2.3.7. of the REACH Regulation. The Registrant is requested to submit the missing information.

2) Missing information related to endpoints

Pursuant to Articles 10(a)(vi), 12(1)(d) of the REACH Regulation, a registration for a substance produced in quantities of [redacted] shall contain [redacted] the information specified in Annexes VII and VIII of the REACH Regulation.

2.1) Boiling point

The technical dossier contained: 1) the result of an experimental study and 2) a qualitative or quantitative structure-activity relationship model (QSAR) estimate both with reliability 4 (not assignable) according to Klimisch classification.
The information provided does not meet the information requirement for this endpoint for the following reasons:

1) Experimental study. The technical dossier contains only few details of how the experimental study has been performed. In order to allow an independent assessment of the endpoint including reliability and completeness, the study summary for this endpoint needs to contain pressure value and unit, rate of temperature increase, decomposition (if applicable), accuracy and boiling point value in °C, corrected to standard pressure. These elements are missing in the technical dossier, and therefore it is not possible to evaluate the validity of the study. The shortcomings of this study are reflected in the reliability score of 4 (not assignable), assigned by the Registrant;
2) QSAR study. Annex XI, section 1.3 sets out conditions which are a prerequisite for acceptance of a QSAR prediction. These conditions are not met because no information was provided to prove that the substance falls within the applicability domain of the QSAR model, and no adequate and reliable documentation of the applied method has been provided. Consequently it is not possible to evaluate the validity of this QSAR study. The shortcomings of this study are reflected in the reliability score of 4 (not assignable), assigned by the Registrant.

Because no adequate and reliable information exists on this endpoint, the Registrant is requested to submit the information for this endpoint using the test method A.2 of Regulation (EC) No 440/2008 and to update the technical dossier and the Chemical Safety Report (CSR) with the relevant information.

2.2) Vapour pressure

The technical dossier contained: 1) the result of an experimental study with reliability 3 (not reliable) and 2) a QSAR estimate using EPISUITE with reliability 4 (not assignable) according to Klimisch classification.
The information provided does not meet the requirement for this endpoint for the following reasons:

1) Experimental study. The technical dossier contains only few details of how the experimental study has been performed. In order to allow an independent assessment of the endpoint including reliability and completeness, the robust study summary for this endpoint should also contain type of method used, estimates of the vapour pressure at 20 or 25 °C and accuracy. These elements are missing in the technical dossier, and therefore it is not possible to evaluate the validity of the study. The shortcomings of this study are reflected in the reliability score of 3 (not reliable), assigned by the Registrant;
2) QSAR study. Annex XI, section 1.3 sets out conditions which are a prerequisite for acceptance of a QSAR prediction. These conditions are not met because no information was provided to prove that the substance falls within the applicability domain of the QSAR model, and no adequate and reliable documentation of the applied method has been provided. Consequently it is not possible to evaluate the validity of this QSAR study. The shortcomings of this study are reflected in the reliability score of 4 (not assignable), assigned by the Registrant;
3) The experimental result and the QSAR prediction provide conflicting results. The QSAR model predicts a vapour pressure of 0.226mm Hg (30 Pa) at 25 °C, whereas the experimental study indicates a much lower vapour pressure of 1.2 Pa at a higher temperature (68 °C).

The estimate of vapour pressure is important for determining the exposure of workers to the registered substance. The risk assessment is based upon the exposure estimates, and may be critically affected by the value of the vapour pressure estimate. Therefore, the Registrant is requested to submit the information for this endpoint using the test method A.4 of Regulation (EC) No 440/2008 and to update the technical dossier and the CSR with the relevant information.

2.3) Auto-ignition temperature

The technical dossier contained: 1) the result of an experimental study with reliability 3 (not reliable) according to Klimisch classification and 2) statements for the use of a read-across approach from a supporting substance (structural or analogue surrogate) for the registered substance based on structural similarity.
The information provided does not meet the requirement for this endpoint for the following reasons:

1) Experimental study. The technical dossier contains only few details of how the experimental study has been performed. In order to allow an independent assessment of the endpoint including reliability and completeness, the robust study

summary for this endpoint should also contain quantity of sample used, apparatus used, temperature/time curve, pressure, and accuracy. These elements are missing in the technical dossier, and therefore it is not possible to evaluate the validity of the study;

2) Read-across. The technical dossier contains the result of an auto-ignition temperature study (EU Method A.15) for vinyl neodecanoate as a structural analogue for vinyl neononanoate. Annex VIII, second introductory paragraph, requires the Registrant to clearly state reasons for adapting the standard information requirements according to the rules in Annex XI. As insufficient justification was provided for read-across, the requirements of Annex XI, Section 1.5 in conjunction with Annex VIII, second introductory paragraph, of the REACH Regulation were not met. Specifically, although the substance shares common functional groups to the read-across substance, the identities of both the registered substance and the read-across substance are unclear. Additionally, it is not possible to establish a constant pattern in the changing potency of this property for these substances. Finally, read-across may not be appropriate for this endpoint as the auto-ignition temperature can vary significantly based on small changes in the substance's structure. This can be seen from comparing the result of the experimental study for vinyl neodecanoate, which indicates an auto-ignition temperature of 267-279 °C, and the above experimental study for the registered substance, which shows an auto-ignition temperature of 372 °C. On this basis, vinyl neodecanoate fails the requirement of Annex XI, 1.5 and so the read-across to vinyl neononanoate is not justified.

Therefore, the Registrant is accordingly requested to submit the information for this endpoint using the test method A.15 of Regulation (EC) No 440/2008 and to update the technical dossier and the CSR with the relevant information.

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

ECHA reminds registrants of the requirements of Article 13(4) of the REACH Regulation that ecotoxicological and toxicological tests and analyses shall be carried out in compliance with the principles of good laboratory practice (GLP).

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 or to other international test methods recognised as being appropriate and use the applicable test methods to generate the information on the endpoints indicated above.

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 internet page at http://echa.europa.eu/appeals/app_procedure_en.asp. The notice of appeal will be deemed to be filed only when the appeal fee has been paid.

[redacted]

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Director of Regulatory Affairs