EUROPEAN CHEMICALS AGENCY

Helsinki, 11 June 2020

Addressees
Registrant of JS_S_ISOBUTYL_XANTHATE listed in the last Appendix of this decision

Date of submission for the dossier subject of this decision
25 April 2018

Registered substance subject to this decision, hereafter 'the Substance'
Substance name: Sodium O-isobutyl dithiocarbonate
EC number: 246-805-2
CAS number: 25306-75-6

Decision number: [Please refer to the REACH-IT message which delivered this communication (in format CCH-D-XXXXXXXXXX-XX-XX/D)]

DECISION ON A COMPLIANCE CHECK

Based on Article 41 of Regulation (EC) No 1907/2006 (REACH), ECHA requests that you submit the information listed below by the deadline of ***16 September 2022***.

A. Requirements applicable to all the Registrants subject to Annex VI of REACH

1. Spectral data (Annex VI, Section 2.3.5.) and high-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.);

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

B. Requirements applicable to all the Registrants subject to Annex VII of REACH

1. Surface tension (Annex VII, Section 7.6.; test method: EU A.5./OECD TG 115) with the Substance;

2. Water solubility (Annex VII, Section 7.7.; test method: EU A.6./OECD TG 105 with the Substance;

3. Partition coefficient n-octanol/water (Annex VII, Section 7.8.; using an appropriate test method) with the Substance;

4. In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.; test method EU B.13/14. / OECD TG 471) with the Substance;

5. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.; test method EU C.2./OECD TG 202) with the Substance;

6. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.; test method EU C.3./OECD TG 201) with the Substance;

C. Requirements applicable to all the Registrants subject to Annex VIII of REACH

1. In vitro cytogenicity study in mammalian cells (Annex VIII, Section 8.4.2., test method OECD TG 473) or in vitro micronucleus study (Annex VIII, Section 8.4.2., test method OECD TG 487) with the Substance;

2. Only if a negative result in Annex VII, Section 8.4.1. and Annex VIII, Section 8.4.2. is obtained, In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.; test method OECD TG 476 or TG 490) with the Substance;

3. Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.; test method OECD TG 203) with the Substance;

D. Requirements applicable to all the Registrants subject to Annex IX of REACH

1. Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.; test method OECD TG 408) in rats with the Substance;

2. Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.; test method OECD TG 414) in a first species (rat or rabbit), oral route with the Substance;

3. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.; test method EU C.20./OECD TG 211) with the Substance;

4. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.; test method OECD TG 210) with the Substance.

The assessment and reasoning for requests B.4, C.1-2, and D.1-2 is based on the jointly submitted information in the Lead registrant's dossier, and they are identical to the requests in a decision addressed to the relevant members of the Joint submission. However, they are included in this decision due to partial opt-out by you.

Conditions to comply with the requests

You are bound by the requests for information corresponding to the REACH Annexes applicable to your registered tonnage of the Substance at the time of evaluation of the dossier. You have to comply with the requirements of Annexes VI-IX of REACH, if you have registered a substance at 100-1000 tpa.

Registrants are only required to share the costs of information that they must submit to fulfil the information requirements for their registration.

The Appendix on general considerations addresses issues relevant for several requests while the other Appendices state the reasons for the requests for information to fulfil the requirements set out in the respective Annexes of REACH.

The Appendix entitled Observations and technical guidance addresses the generic approach for the selection and reporting of the test material used to perform the required studies and provides generic recommendations and references to ECHA guidance and other reference documents.

You must submit the information requested in this decision by the deadline indicated above in an updated registration dossier and also update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information. The timeline has been set to allow for sequential testing where relevant.

Appeal

This decision can be appealed to the Board of Appeal of ECHA within three months of its notification. An appeal, together with the grounds thereof, has to be submitted to ECHA in writing. An appeal has suspensive effect and is subject to a fee. Further details are described under: http://echa.europa.eu/regulations/appeals.

Approved[1] under the authority of Christel Schilliger-Musset, Director of Hazard Assessment

[1] As this is an electronic document, it is not physically signed. This communication has been approved according to ECHA's internal decision-approval process.

Appendix on general considerations

(i) Assessment of the QSAR adaptations, under the requirements of Annex XI, Section 1.3.

You have adapted the following standard information requirements by applying QSAR approach in accordance with Annex XI, Section 1.3:

- Water solubility (Annex VII, Section 7.7.)
- Partition coefficient n-octanol/water (Annex VII, Section 7.8.)
- In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.)
- In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)
- In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)
- Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)

We have assessed this information and identified the following general issues:

For the use of QSAR models under Annex XI, Section 1.3. of REACH, the following cumulative conditions shall be necessarily met: results are derived from a (Q)SAR model whose scientific validity has been established; the substance falls within the applicability domain of the model; results are adequate for the purpose of classification and labelling and/or risk assessment; adequate and reliable documentation of the applied method is provided.

According to ECHA's Practical guide "How to use and report (Q)SARs", section 3.4, a QSAR Model Reporting Format (QMRF) and a QSAR Prediction Reporting Format (QPRF) are required to establish the scientific validity of the model, to verify that the Substance falls within the applicability domain of the model, and to assess the adequacy of the prediction for the purposes of classification and labelling.

However, the information you have provided does not meet the cumulative conditions mentioned above. The Substance does not fall within the applicability domain of the model (see ECHA Guidance R.6, Section R.6.1.5, and ECHA's Practical guide "How to use and report (Q)SARs", section 3.2) because the Substance has a dithiocarbonate functional group, which is not covered by the training set of the applied model either in its acidic or anionic form. Therefore, the results are inadequate for classification and labelling and/or risk assessment.

Although documentation was provided for toxicological endpoints, you have not provided any documentation for the QSAR predictions on the physical-chemical or environmental endpoints (in particular, you have not included a QMRF and/or a QPRF in your technical dossier).

Therefore, the results are inadequate for classification and labelling and/or risk assessment. Consequently, the adaptations are rejected.

(ii) Assessment of the Grouping of substances and read-across approach, under the requirements of Annex XI, Section 1.5.

You have adapted the following standard information requirements by applying read-across approaches in accordance with Annex XI, Section 1.5:

- Short-term toxicity testing on aquatic invertebrates (Annex VII, Section 9.1.1.)
- Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)
- Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.)

- Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.)

ECHA has considered the scientific and regulatory validity of your read-across approach in general before assessing the specific standard information requirements in the following appendices.

Grouping of substances and read-across approach

Annex XI, Section 1.5. of REACH specifies two conditions which must be fulfilled whenever a read-across approach is used. Firstly, there needs to be structural similarity between substances which results in a likelihood that the substances have similar physicochemical, toxicological and ecotoxicological properties so that the substances may be considered as a group or category. Secondly, it is required that the relevant properties of a substance within the group may be predicted from data for reference substance(s) within the group. Additional information on what is necessary when justifying a read-across approach can be found in the ECHA Guidance R.6 and the ECHA RAAF document.

You read-across between the structurally similar (source) substances and the Substance as target substance. You used the following source substances:

- sodium O-isopropyl dithiocarbonate EC No. 205-443-5 (CAS No. 140-93-2) for short-term toxicity testing on fish and aquatic invertebrates and long-term toxicity testing on aquatic invertebrates; and
- potassium O-pentyl dithiocarbonate EC No. 220-329-5 (CAS No. 2720-73-2) for long-term toxicity testing on fish.
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You indicate that these substances belong to a group of "xanthates". According to the information provided in your Chemical Safety Report, "The group of the compounds is called xanthates, derived from the xanthate radical: [redacted] They are products of a reaction between carbon disulfide, relevant alcohol and sodium or potassium hydroxide. Each of the substance: contain common functional group – [redacted] decomposes via physical and biological processes to common products: carbon disulfide, an alcohol and alkali hydroxide, is characterized by a constant pattern in the changing of the properties across the category."

ECHA understands from this information that you intend to predict the properties of the Substance using a read-across hypothesis which assumes that different compounds have the same type of effects. The properties of your Substance are predicted to be quantitatively equal to those of the source substance.

ECHA notes the following general shortcomings with regards to prediction of ecotoxicological properties. Specific considerations regarding individual endpoints, which also result in a failure to meet the requirement of Annex XI, 1.5, are set out under the concerned endpoint-specific sections in the following Appendices.

1. Missing information on the composition of the source substances

Annex XI, Section 1.5 of REACH provides that "*substances whose physicochemical, toxicological and ecotoxicological properties are likely to be similar or follow a regular pattern as a result of chemical similarity may be considered as group.*"

According to the ECHA Guidance, "*the purity and impurity profiles of the substance and the structural analogue need to be assessed*", and "*the extent to which differences in the purity*

and impurities are likely to influence the overall toxicity needs to be addressed, and where technically possible, excluded". The purity profile and composition can influence the overall toxicity/properties of the Substance and of the source substance(s).[2] Therefore, qualitative and quantitative information on the compositions of the Substance and of the source substance(s) should be provided to allow assessment whether the attempted predictions are compromised by the composition and/or impurities.

In your technical dossier you have described the source substances only by its EC and CAS numbers, but no information on the composition of this substance is reported.

Without detailed information on the composition of the source substances, no qualitative or quantitative comparative assessment of the compositions of the Substance and of the source substances can be completed. Therefore, ECHA considers that it is not possible to assess whether the attempted predictions are compromised by the composition of the source substances.

2. Missing supporting information

Annex XI, Section 1.5 of REACH states that "*physicochemical properties, human health effects and environmental effects or environmental fate may be predicted from data for reference substance(s)*". For this purpose "*it is important to provide supporting information to strengthen the rationale for the read-across*"[3]. The set of supporting information should allow to verify the crucial aspects of the read-across hypothesis and establish that the properties of the Substance can be predicted from the data on the source substance(s).

Supporting information must include supporting information/bridging studies to compare properties of the Substance and source substance(s).

As indicated above, your read-across hypothesis is based on the assumption that the structurally similar substances cause the same type of effect(s). In this context, relevant, reliable and adequate information allowing to compare the properties of the Substance and of the source substance(s) is necessary to confirm that the substances cause the same type of effects. Such information can be obtained, for example, from bridging studies of comparable design and duration for the Substance and of the source substance(s).

The data set reported in the technical dossier does not include relevant, reliable and adequate information for the Substance and of the source substance(s) to support your read-across hypothesis. In the absence of such information, you have not established that the Substance and of the source substance(s) are likely to have similar properties. Therefore you have not provided sufficient supporting information to strengthen the rationale for the read-across.

3. Source studies not meeting Annex XI Requirements

Annex XI, Section 1.5., if the grouping concept is applied then in all cases the results to be read across should have adequate and reliable coverage of the key parameters addressed in the corresponding test method referred to in Article 13(3).

None of the source studies that you have used in your read-across approach, include any critical supporting information such as study design details, a description of the test solution preparation and other key parameters allowing to assess the validity of the test method applied. In the absence of this information, the results of these studies are considered

[2] ECHA Guidance R.6, Section R.6.2.3.1
[3] ECHA Guidance R.6, Section R.6.2.2.1.f

unreliable.

Conclusions on the read-across approach

As explained above, you have not established that relevant properties of the Substance can be predicted from data on the analogue substance. Therefore, your adaptations do not comply with the general rules of adaptation as set out in Annex XI, Section 1.5. and your grouping and read-across approaches are rejected.

(iii) Assessment of the weight-of-evidence adaptations, under the requirements of Annex XI, Section 1.2.

You have adapted the following standard information requirements by applying weight-of-evidence (WoE) approaches:

- In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.)
- In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)
- Sub-chronic toxicity study (90-day), (Annex IX, Section 8.6.2.)
- Pre-natal developmental toxicity study (Annex IX and X, Section 8.7.2.)

Your WoE adaptations are based on information on the Substance and/or similar substance(s), which you consider a group of xanthates, obtained through the use of data from the QSAR models and/or directly from information on similar substances from the public literature. The individual study records are mentioned under the relevant endpoints in the following Appendices to this decision.

We have assessed this information according to the requirements of Annex XI, Section 1.2 of the REACH Regulation and identified the following general issues with all of these adaptations:

1. Requirement for documentation of the WoE adaptations

Annex XI, Section 1.2 states that there may be sufficient weight of evidence (WoE) from several independent sources of information leading to assumption/conclusion that a substance has or has not a particular dangerous (hazardous) property, while information from a single source alone is insufficient to support this notion. ECHA Guidance R.4.4 specifies that a WoE adaptation must involve an assessment of the relative values / weights of the several pieces of available information. This assessment must consider for instance the relevance and reliability of the information, the consistency of results/data, the nature and severity of effects. The lines of evidence should be integrated considering their relative values or weights in order to draw a conclusion. The assessment should be documented and included in your technical dossier.

However, you have not included a justification for your WoE adaptations, which would include an assessment of relative weights of the individual pieces of information and the subsequent conclusions drawn.

2. Reliability of the experimental information

ECHA Guidance R.4, Section R.4.2 informs on the criteria for assessing the reliability of information provided as part of WoE adaptations. The availability of raw data from the studies and an adequate description of the studies are listed among the key elements to be assessed to determine if and how the information can be used in the adaptation. This ECHA Guidance

indicates that "*where critical supporting information is not reported (e.g. species tested, substance identity and dose procedure) the test data should be considered to be unreliable for the purposes of REACH*".

None of the study summaries provided by you, performed either on the Substance or an analogue substance, include any critical supporting information such as study design details, a description of the test solution preparation or other key parameters allowing to assess the validity of the test method applied. In the absence of this information the results of these studies referred to in your WoE adaptations are considered unreliable.

3. Relevance and reliability of the QSAR information

Whenever sources of information derived from QSAR predictions are used as part of a WoE, the following cumulative conditions shall be necessarily met: results are derived from a (Q)SAR model whose scientific validity has been established; the substance falls within the applicability domain of the model; results are adequate for the purpose of classification and labelling and/or risk assessment; adequate and reliable documentation of the applied method is provided.

According to ECHA's Practical guide "How to use and report (Q)SARs", section 3.4, a QSAR Model Reporting Format (QMRF) and a QSAR Prediction Reporting Format (QPRF) are required to establish the scientific validity of the model, to verify that the Substance falls within the applicability domain of the model, and to assess the adequacy of the prediction for the purposes of classification and labelling.

For toxicological endpoints, you have provided QSAR model prediction reports detailing the structural and mechanistic criteria used for identifying the similar substances and providing high level information on the identity of these substances. We have assessed this information and conclude that the Substance does not fall within the applicability domain because the Substance has a dithiocarbonate functional group, which is not covered by the training set of the applied model either in its acidic or anionic form. Furthermore, the output also mentions that the fragment C(S)-O present in the Substance is similar to a known biophore C(S)-N, and therefore the Substance should be tested experimentally.

4. Relevance of information – requirement for a scientific justification for the use of information from similar substances

Based on the ECHA Guidance R.4, Section R.4.3.2.2., a scientific justification needs to establish why the toxicological or ecotoxicological properties of the Substance can be determined from information on similar substances. It should also explain why the differences between these substances should not influence the toxicological/ecotoxicological properties of the Substance or should do so in a regular predictable pattern.

You have provided information on multiple similar substances. Details on the identity of these substances and on the nature of the information are provided in the endpoint sections in the next Appendices. In order to justify the use of relevance of this information in order to identify the properties of the Substance you have indicated in Part B Section 1.3 of your Chemical Safety Report (CSR) that the substances share structural similarities and decompose via physical and biological processes to common products: carbon disulfide, an alcohol and alkali hydroxide. Your justification refers to the formation of common products via physical and biological processes. However you have not provided any qualitative and quantitative information characterising these processes to support your claim of formation of common products. In the absence of such information you have not established why the toxicological

properties of the Substance can be determined from information on these similar substances. Consequently, this information cannot be considered as relevant for the purpose of identification of the hazard of the Substance by means of weight of evidence.

Conclusion of the WoE assessment

For the reasons presented above, as your WoE adaptations are neither based on data which allowing a conclusion on the relevant hazard properties of the Substance nor supported by adequate documentation, they do not comply with the general rules of adaptation as set out in Annex XI, Section 1.2. Therefore, your adaptations are rejected.

Appendix A: Reasons for the requests to comply with Annex VI of REACH

Under Article 10(a)(ii) of the REACH Regulation, the technical dossier must contain information on the identity of the substance as specified in Annex VI, Section 2 to the REACH Regulation. In accordance with Annex VI, Section 2 the information provided has to be sufficient to enable the identification of the registered substance.

1. Spectral data (Annex VI, Section 2.3.5.)

Spectral data are a formal information requirement as laid down in Annex VI, Section 2.3.5 of the REACH Regulation. Adequate information needs to be present in the technical dossier to meet this information requirement.

The registration dossier does not contain an ultra-violet (UV) spectrum, infra-red (IR) spectrum, nuclear magnetic resonance (NMR) spectrum (or alternatively to this last one a mass spectrum (MS)) performed on the substance. A justification for waiving this information requirement is not given.

Therefore, the information requirement under Annex VI, Section 2.3.5. is not fulfilled and without the missing spectra it is not possible to verify the identity of the substance.

You are requested to submit a UV, IR and NMR (or MS spectra) to confirm the identity of the substance. You shall ensure that the description of the analytical methods used for recording the spectra is specified in the dossier in such detail to allow the methods to be reproduced, in line with the requirements under Annex VI Section 2.3.7 of the REACH Regulation. You will ensure that the information is consistent with the information provided throughout the dossier.

The requested spectral data (and relative method descriptions) shall be attached in section 1.4 of the IUCLID dossier.

2. High-pressure liquid chromatogram, gas chromatogram (Annex VI, Section 2.3.6.)

The provision of a high-pressure liquid chromatogram or gas chromatogram is an information requirement as laid down in Annex VI, Section 2.3.6. of the REACH Regulation. Adequate information needs to be present in the technical dossier to meet this information requirement.

The registration dossier does not contain any chromatographic data that would allow to determine the composition of the substance and consequently its identity. A justification for waiving this information requirement is not given.

Therefore, the information requirement under Annex VI, Section 2.3.6. is not fulfilled and without the missing chromatographic data it is not possible to verify the identity of the substance.

You are requested to submit a chromatogram (e.g. High-pressure liquid chromatogram, gas chromatogram, etc.) for the quantification of the constituents of the substance. The chromatogram shall be accompanied by a peak table including peak position, area, mass percent and the assignment given. The information shall indicate how the chromatogram is supporting the identification of the registered substance as reported in sections 1.1 and 1.2 of the registration dossier. You should also provide a description of the analytical methods

used for the quantification of the registered substance. 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, in line with the requirements under Annex VI Section 2.3.7 of the REACH Regulation. You shall ensure that the information is consistent with the information provided throughout the dossier.

The requested chromatographic data (and relative method descriptions) shall be attached in section 1.4 of the IUCLID dossier.

Appendix B: Reasons for the requests to comply with Annex VII of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier registered at 1 to 10 tonnes or more per year must contain, as a minimum, the information specified in Annex VII to REACH.

1. Surface tension (Annex VII, Section 7.6.)

Surface tension is a standard information requirement in Annex VII to REACH.

You have adapted this information requirement with the following statement: "*Study is technically not feasible*" and "*The study does not need to be conducted because surface activity is not a desired property of the material.*"

According to Annex XI, Section 2, testing for a specific endpoint may be omitted, if it is technically not possible to conduct the study as a consequence of the properties of the Substance. However, besides the above statement you have not provided any evidence why testing for the Substance would not be technically possible. ECHA can therefore not verify whether and why it is technically not possible to conduct the study as a consequence of the properties of the Substance.

According to Annex VII, Section 7.6, Column 2, the study need only be conducted if, a) based on structure, surface activity is expected or can be predicted, or b) surface activity is a desired property of the material. However, the adaptation provided by you (surface tension is not a desired property of the material) does not exclude the need for testing on the basis of the information provided by you, because based on the structure of the Substance, surface activity can be expected. In particular, the Substance has hydrophilic and lipophilic moieties.

Therefore, your adaptations based on Annex XI, Section 2 and Annex VII, Section 7.6, Column 2 are rejected and the information requirement is not fulfilled.

2. Water solubility (Annex VII, Section 7.7.)

Water solubility is a standard information requirement in Annex VII to REACH.

You have adapted this information requirement based on Annex XI, Section 1.3 of REACH (QSAR).

You have provided a calculated value for this endpoint. You have reported an estimation of the water solubility of the Substance based on EPISuite prediction software. You report the water solubility of the Substance to be 662.6 mg/l at 25 °C and pH 7.

You have not provided a QMRF and a QPRF for your prediction. As explained in the Appendix on general considerations section (i), in the absence of this information your adaptation is rejected because ECHA cannot verify that the cumulative conditions of Annex XI, Section 1.3 are met. Your adaptation does not comply with the general rules of adaptation as set out in Annex XI, Section 1.3. Therefore, your adaptation is rejected and the information requirement is not fulfilled.

Possibility for data sharing:
The jointly submitted registration for the Substance contains data which is relevant for this endpoint. In accordance with Title III of the REACH Regulation, you may request it from the other registrant(s) and then make every effort to reach an agreement on the sharing of data

and costs[4].

3. Partition coefficient n-octanol/water (Annex VII, Section 7.8.)

Partition coefficient n-octanol/water is a standard information requirement in Annex VII to REACH. You have adapted this information requirement based on Annex XI, Section 1.3 of REACH (QSAR).

You have provided a calculated value for this endpoint. You have reported an estimation of the partition coefficient *n*-octanol/water of the Substance based on EPISuite software. You report the partition coefficient of the Substance to be -1.33 at 20 °C and pH 7.

You have not provided a QMRF and a QPRF for your prediction. As explained in the Appendix on general considerations section (i), in the absence of this information your adaptation is rejected because ECHA cannot verify that the cumulative conditions of Annex XI, Section 1.3 are met.

Therefore, the information requirement is not fulfilled.

Possibility for data sharing:

The jointly submitted registration for the Substance contains data which is relevant for this endpoint. In accordance with Title III of the REACH Regulation, you may request it from the other registrant(s) and then make every effort to reach an agreement on the sharing of data and costs[4].

4. In vitro gene mutation study in bacteria (Annex VII, Section 8.4.1.)

An *In vitro* gene mutation study in bacteria is a standard information requirement in Annex VII to REACH.

You have adapted the standard information requirement according to Annex XI, Section 1.2. Weight of evidence of REACH. In support of this adaptation of the information requirement, you have provided the following information for this endpoint:

i. With analogue substance carbon disulphide (CAS: 75-15-0, EC: 200-843-6), U.S. Department of Health and Human Services, 1996 - *in vitro* gene mutation study in bacteria, similar to OECD Test Guideline 471;

ii. Information obtained from QSAR prediction (2012) on the Substance, A7A-A7E from FDA Genetic toxicity set. Model: MC4PC version 2.4.1.5c.

We have assessed this information according to the requirements of Annex XI, Section 1.2 of the REACH Regulation and identified the following issue(s):

As explained in the Appendix on general considerations (iii) (1, 2, 3, 4) your adaptation is rejected, because of shortcomings of the study summaries, unreliablity of the QSAR information, and a lack of supporting information establishing why the toxicological properties of the Substance can be determined from information on the similar substance(s).

Therefore, the information requirement is not fulfilled.

5. Short-term toxicity testing on aquatic invertebrates (Annex VII, Section

[4] ECHA Guidance on data-sharing

9.1.1.)

Short-term toxicity testing on aquatic invertebrates is a standard information requirement in Annex VII to REACH.

You have adapted this information requirement by using a read-across approach under Annex XI, Section 1.5. You have provided:

i. a key study (1978) on analogue substance (sodium O-isopropyl dithiocarbonate; EC No. 205-443-5, CAS No. 140-93-2), performed according to OECD TG 202.

As explained in the Appendix on general considerations (ii) (1 and 2) your adaptation is rejected because of the lack of information on characterisation of the source substance and lack of supporting information establishing why the ecotoxicological properties of the Substance can be determined from information on the similar substances.

Therefore, the information requirement is not fulfilled.

6. Growth inhibition study aquatic plants (Annex VII, Section 9.1.2.)

Growth inhibition study aquatic plants is a standard information requirement in Annex VII to REACH. You have adapted this information requirement based on Annex XI, Section 1.3 of REACH (QSAR).

You have provided a calculated value for this endpoint.You have reported an estimation of the toxicity to aquatic plants of the Substance based on ECOSAR software. You report the EC50 of the Substance to be 74.6 mg/L.

You have not provided a QMRF and a QPRF for your prediction. As explained in the Appendix on general considerations section (i), in the absence of this information your adaptation is rejected because ECHA cannot verify that the cumulative conditions of Annex XI, Section 1.3 are met.

Therefore, the information requirement is not fulfilled.

Appendix C: Reasons for the requests to comply with Annex VIII of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier registered at 10 to 100 tonnes or more per year must contain, as a minimum, the information specified in Annexes VII and VIII to REACH.

1. In vitro cytogenicity study in mammalian cells or in vitro micronucleus study (Annex VIII, Section 8.4.2.)

An *In vitro* cytogenicity study in mammalian cells or an *In vitro* micronucleus study is a standard information requirement in Annex VIII to REACH.

You have adapted the standard information requirement according to Annex XI, Section 1.2. Weight of evidence of REACH.

In support of this adaptation of the information requirement, you have provided the following information for this endpoint:

i. Information obtained from QSAR prediction on the Substance, *in vitro* cytogenicity / chromosome aberration study (2012) on the Substance, A7U-A7X and A8H from FDA Genetic toxicity set. Model version: MC4PC version 2.4.1.5;

ii. Information obtained from QSAR prediction on the Substance, genetic toxicity *in vitro*.ToxTree: Benigni/Bossa rules for carcinogenicity and mutagenicity.

We have assessed this information according to the requirements of Annex XI, Section 1.2 of the REACH Regulation and as explained in the Appendix on general considerations section (iii) (1, 3) your adaptation is rejected.

Therefore, the information requirement is not fulfilled.

2. In vitro gene mutation study in mammalian cells (Annex VIII, Section 8.4.3.)

An *in vitro* gene mutation study in mammalian cells is a standard information requirement in Annex VIII to REACH in case of a negative result in the *in vitro* gene mutation test in bacteria and the *in vitro* cytogenicity test.

You have adapted the standard information requirement according to Annex XI, Section 1.3. QSAR of REACH.

In support of this adaptation of the information requirement, you have provided the following information for this endpoint:

i. Information obtained from QSAR prediction on the Substance, *in vitro* gene mutation study in mammalian cells, Model name: A7O, A7N, AN7 and AN8 from FDA Genetic toxicity set Model version: MC4PC version 2.4.1.5.

We have assessed this information according to the requirements of Annex XI, Section 1.3 of the REACH Regulation and as explained in the Appendix on general considerations section (i) your adaptation is rejected.

Therefore, the information requirement is not fulfilled.

3. Short-term toxicity testing on fish (Annex VIII, Section 9.1.3.)

Short-term toxicity testing on fish is a standard information requirement in Annex VIII to REACH.

You have adapted this information requirement by using a read-across approach under Annex XI, Section 1.5. You have provided:

i. a key study (1974) on analogue substance (sodium O-isopropyl dithiocarbonate, EC No. 205-443-5, CAS No. 140-93-2), performed according to OECD TG 203.

As explained in the Appendix on general considerations (ii) (1 and 2) your adaptation is rejected because of the lack of information on characterisation of the source substance and lack of supporting information establishing why the ecotoxicological properties of the Substance can be determined from information on the similar substances.

Therefore, the information requirement is not fulfilled.

Appendix D: Reasons for the requests to comply with Annex IX of REACH

Under Articles 10(a) and 12(1) of REACH, a technical dossier registered at 100 to 1000 tonnes or more per year must contain, as a minimum, the information specified in Annexes VII to IX to REACH.

1. Sub-chronic toxicity study (90-day), oral route (Annex IX, Section 8.6.2.)

A Sub-chronic toxicity study (90 day) is a standard information requirement in Annex IX to REACH.

You have adapted the standard information requirement according to Annex XI, Section 1.2. Weight of evidence of REACH.

In support of this adaptation of the information requirement, you provided the following information from analogue substance for this endpoint, three oral studies and seven inhalation studies:

i. Australian Government Publishing Service Canberra, 1995, Potassium butyl xanthate (CAS No: 871-58-9 EC No: 212-808-2), similar to OECD Test Guideline 408 (Repeated Dose 90-Day Oral Toxicity in rats);
ii. Canadian Centre for Occupational Health and Safety Year, 2010, Potassium ethyl xanthate (CAS No: 140-89-6 EC No: 205-439-3), no guideline mentioned;
iii. U.S. Department of Health and Human Services Year 1996, Carbon disulfide (CAS No: 75-15-0 EC No: 200-843-6) similar to OECD Test Guideline 407 (Repeated Dose 28-Day oral Toxicity in rats);
iv. Australian Government Publishing Service Canberra, 1995, Potassium amyl xanthate (CAS No: 2720-73-2 EC No: 220-329-5), similar to OECD Test Guideline 412 (Subacute Inhalation Toxicity: 28-Day Study in mice);
v. Australian Government Publishing Service Canberra, 1995, Potassium amyl xanthate (CAS No: 2720-73-2 CAS No: 220-329-5), similar to OECD Test Guideline 412 (Subacute Inhalation Toxicity: 28-Day Study in rats);
vi. Australian Government Publishing Service Canberra, 1995, Potassium amyl xanthate (CAS No: 2720-73-2 EC No: 220-329-5), similar to OECD Test Guideline 412 (Subacute Inhalation Toxicity: 28-Day Study in rabbits);
vii. Australian Government Publishing Service Canberra, 1995, Potassium amyl xanthate (CAS No: 2720-73-2 EC No: 220-329-5), similar to OECD Test Guideline 412 (Subacute Inhalation Toxicity: 28-Day Study in dogs);
viii. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6), no guideline mentioned;
ix. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6), similar to OECD Test Guideline 413 (Subchronic Inhalation Toxicity: 90-Day Study in rats);
x. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6), similar to OECD Test Guideline 413 (Subchronic Inhalation Toxicity: 90-Day Study in mice).

We have assessed this information according to the requirements of Annex XI, Section 1.2 of the REACH Regulation and, as explained in the Appendix on general considerations (iii) (1, 2, 4), your adaptation is rejected because of shortcomings of the study summaries and a lack of supporting information establishing why the toxicological properties of the Substance can be determined from information on the similar substances.
Therefore, the information requirement is not fulfilled.

Referring to the criteria provided in Annex IX, Section 8.6.2, Column 2, the oral route is the most appropriate route of administration to investigate repeated dose toxicity, because the Substance is a solid and is used as such with low dustiness. The use information provided in the Chemical Safety Report indicates that human exposure to the Substance by the inhalation route is unlikely.

Therefore the sub-chronic toxicity study must be performed according to the OECD TG 408, in rats and with oral administration of the Substance.

2. Pre-natal developmental toxicity study (Annex IX, Section 8.7.2.) in a first species

A Pre-natal developmental toxicity (PNDT) study (OECD TG 414) in one species is a standard information requirement under Annex IX to REACH.

You have adapted the standard information requirement according to Annex XI, Section 1.2 (Weight of evidence).

In support of this adaptation of the information requirement, you provided the following information from analogue substance for this endpoint,

i. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6), similar to OECD Test Guideline 414 (Prenatal Developmental Toxicity Study) inhalation, rabbit;
ii. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6) similar to OECD Guideline 414 (Prenatal Developmental Toxicity Study) oral, rat;
iii. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6) similar to OECD Guideline 414 (Prenatal Developmental Toxicity Study) inhalation, rat;
iv. U.S. Department of Health and Human Services Year 1996, Carbon disulphide (CAS No: 75-15-0 EC No: 200-843-6) similar to OECD Guideline 414 (Prenatal Developmental Toxicity Study) inhalation, mouse.

We have assessed this information according to the requirements of Annex XI, Section 1.2 of the REACH Regulation.

As explained in the Appendix on general considerations (iii) (1, 2 and 4) your adaptation is rejected, because of shortcomings of the study summaries, and a lack of supporting information establishing why the toxicological properties of the Substance can be determined from information on the similar substance(s).

In the absence of this information, the information from studies (i – iv) referred to in your WoE adaptations is considered unreliable.

Therefore, the information requirement is not fulfilled.

A PNDT study according to the test method OECD TG 414 should be performed in rat or rabbit as preferred species with oral administration of the Substance.

3. Long-term toxicity testing on aquatic invertebrates (Annex IX, Section 9.1.5.)

Long-term toxicity testing on aquatic invertebrates is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement by using a read-across approach under Annex XI, Section 1.5. You have provided:

i. a key study (1978) on analogue substance (sodium O-isopropyl dithiocarbonate; EC No. 205-443-5, CAS No. 140-93-2),

As explained in the Appendix on general considerations (ii) (1, 2 and 3) your adaptation is rejected because of the lack of information on characterisation of the source substance, lack of supporting information establishing why the ecotoxicological properties of the Substance can be determined from information on the similar substances and the source studies not meeting Annex XI Requirements. With regards to study (i), the test was not performed according to any recommended test guidelines.

Therefore, the information requirement is not fulfilled.

4. Long-term toxicity testing on fish (Annex IX, Section 9.1.6.1.)

Long-term toxicity testing on fish is a standard information requirement in Annex IX to REACH.

You have adapted this information requirement by using a read-across approach under Annex XI, Section 1.5. You have provided:

i. a key study (1976) on analogue substance (potassium O-pentyl dithiocarbonate; EC No. 220-329-5, CAS No. 2720-73-2),.

As explained in the Appendix on general considerations (ii) (1, 2 and 3) your adaptation is rejected because of the lack of information on characterisation of the source substance, lack of supporting information establishing why the ecotoxicological properties of the Substance can be determined from information on the similar substances and the source studies not meeting Annex XI Requirements. With regards to study (i), the test was not performed according to any recommended test guidelines.

Therefore, the information requirement is not fulfilled.

Appendix E: Procedural history

For the purpose of the decision-making, this decision does not take into account any updates of registration dossiers after the date on which you were notified the draft decision according to Article 50(1) of REACH.

The compliance check was initiated on 14 March 2019.

The decision making followed the procedure of Articles 50 and 51 of the REACH Regulation, as described below:

ECHA notified you of the draft decision and invited you to provide comments within 30 days of the notification.

ECHA did not receive any comments within the 30-day notification period.

ECHA notified the draft decision to the competent authorities of the Member States for proposals for amendment.

As no amendments were proposed, ECHA adopted the decision under Article 51(3) of REACH.

Appendix F: Observations and technical guidance

1. This compliance check decision does not prevent ECHA from initiating further compliance checks at a later stage on the registrations present.

2. Failure to comply with the requests in this decision, or to otherwise fulfil the information requirements with a valid and documented adaptation, will result in a notification to the enforcement authorities of the Member States.

3. Test guidelines, GLP requirements and reporting

   Under Article 13(3) of REACH, all new data generated as a result of this decision needs to be conducted according to the test methods laid down in a European Commission Regulation or according to international test methods recognised by the Commission or ECHA as being appropriate.

   Under Article 13(4) of REACH, ecotoxicological and toxicological tests and analyses shall be carried out according to the GLP principles (Directive 2004/10/EC) or other international standards recognised by the Commission or ECHA.

   Under Article 10 (a) (vi) and (vii) of REACH, all new data generated as a result of this decision must be reported as study summaries, or as robust study summaries, if required under Annex I of REACH. See ECHA Practical Guide: 'How to report robust study summaries'[5].

4. Test material

   Selection of the test material(s)

   The registrants of the Substance are responsible for agreeing on the composition of the test material to be selected for carrying out the tests required by the present decision. The test material selected must be relevant for all the registrants of the Substance, i.e. it takes into account the variation in compositions reported by all members of the joint submission. The composition of the test material(s) must fall within the boundary composition(s) of the Substance.

   While selecting the test material you must take into account the impact of each constituent/ impurity on the test results for the endpoint to be assessed. For example, if a constituent/ impurity of the Substance is known to have an impact on (eco)toxicity, the selected test material must contain that constituent/ impurity.

   Technical reporting of the test material

   The composition of the selected test material must be reported in the respective endpoint study record, under the Test material section. The composition must include all constituents of the test material and their concentration values [and other parameters relevant for the property to be tested, in this case...]. Without such detailed reporting, ECHA may not be able to confirm that the test material is relevant for the Substance and to all the registrants of the Substance.

[5] https://echa.europa.eu/practical-guides

Technical instructions are available in the manual "How to prepare registration and PPORD dossiers"[6].

5. List of references of the ECHA Guidance and other guidance/ reference documents[7]

Evaluation of available information
Guidance on information requirements and chemical safety assessment, Chapter R.4 (version 1.1., December 2011), referred to as ECHA Guidance R.4 in this decision.

QSARs, read-across and grouping
Guidance on information requirements and chemical safety assessment, Chapter R.6 (version 1.0, May 2008), referred to as ECHA Guidance R.6 in this decision.

ECHA Read-across assessment framework (RAAF, March 2017)[8]

Physical-chemical properties
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Toxicology
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

Environmental toxicology and fate
Guidance on information requirements and chemical safety assessment, Chapter R.7a (version 6.0, July 2017), referred to as ECHA Guidance R.7a in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7b (version 4.0, June 2017), referred to as ECHA Guidance R.7b in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.7c (version 3.0, June 2017), referred to as ECHA Guidance R.7c in this decision.

PBT assessment
Guidance on information requirements and chemical safety assessment, Chapter R.11 (version 3.0, June 2017), referred to as ECHA Guidance R.11 in this decision.

Guidance on information requirements and chemical safety assessment, Chapter R.16 (version 3.0, February 2016), referred to as ECHA Guidance R.16 in this decision.

OECD Guidance documents[9]
Guidance Document on aqueous-phase aquatic toxicity testing of difficult test chemicals – No 23, referred to as OECD GD23.

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[6] https://echa.europa.eu/manuals
[7] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment
[8] https://echa.europa.eu/support/registration/how-to-avoid-unnecessary-testing-on-animals/grouping-of-substances-and-read-across
[9] http://www.oecd.org/chemicalsafety/testing/series-testing-assessment-publications-number.htm

Guidance Document on Mammalian Reproductive Toxicity Testing and Assessment – No 43, referred to as OECD GD43.

Guidance on data-sharing (version 3.1, January 2018), referred to as ECHA Guidance on data-sharing in this decision.

Appendix G: List of the registrants to which the decision is addressed and the corresponding information requirements applicable to them

Registrant Name	Registration number	(Highest) Data requirements to be fufilled
[redacted]	[redacted]	[redacted]