~~Confidential~~

Helsinki, 03 November 2021

Addressees
Registrant listed in the last Appendix of this decision

Date of submission of the dossier subject to this decision
05/05/2020

Registered substance subject to this decision ("the Substance")
Substance name: Reaction mass of 2-methylpropan-1-ol and sodium O-isobutyl dithiocarbonate and sodium hydroxide
List number: 904-290-8

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

DECISION ON A COMPLIANCE CHECK

Under Article 41 of Regulation (EC) No 1907/2006 (REACH), you must submit the information listed below, by the deadline of ***10 February 2022***.

1. **Composition of the substance (Annex VI, Section 2.3.);**

2. **Name or other identifier of the Substance (Annex VI, Section 2.1.);**

   - **EC and/or CAS entry, Chemical name**

The reasons of this decision are set out in Appendix A. The procedural history is described in Appendix B.

The scope of this compliance check decision is limited to the standard information requirements of Annex VI, Section 2 of REACH.

How to comply with your information requirements

To comply with your information requirements you must submit the information requested by this decision in an updated registration dossier by the deadline indicated above. You must also update the chemical safety report, where relevant, including any changes to classification and labelling, based on the newly generated information.

Appeal

This decision, when adopted under Article 51 of REACH, may be appealed to the Board of Appeal of ECHA within three months of its notification to you. Please refer to http://echa.europa.eu/regulations/appeals for further information.

Failure to comply

If you do not comply with the information required by this decision by the deadline indicated above, ECHA will notify the enforcement authorities of your Member State.

Authorised[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 A: Reasons to request information required under Annex VI of REACH

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

1. Composition of the substance (Annex VI, Section 2.3.)

"Composition of the substance" is an information requirement as laid down in Annex VI, Section 2.3 of the REACH Regulation. Adequate information needs to be present in the technical dossier for the registered substance to meet this information requirement.

a. Some of the reported "main constituents" are actually solvents which can be separated

Under Article 3 of the REACH Regulation and Article 2 of the CLP Regulation, a substance is "*a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition*".

According to this definition, solvents which may be separated without affecting the stability of the substance or changing its composition must not be taken into account in the identification of a substance and when making the mass balance. The "Guidance for identification and naming of substances under REACH and CLP" (Version 2.1 - May 2017), referred thereinafter as the "SID guidance", available on the ECHA website[2], explains that in case a solvent is also acting as stabilizing agent and cannot be totally separated due to the properties of the substance, the solvent has to be regarded as an additive and not as a solvent only. In its role of additive, this solvent is an essential constituent of the substance and must be taken into account when making the mass balance. In the role of additive, the solvent does not contribute to the naming of the substance and its identification.

In IUCLID section 1.2, you have reported, among others, the following constituents:

- 2-methylpropan-1-ol, with typical concentration >[redacted]% (w/w) and concentration ranges [redacted]% (w/w);
- Water, with typical concentration <[redacted]% (w/w) and concentration ranges [redacted]% (w/w);

According to the description of the manufacturing process included in IUCLID section 1.2, and on the base of the chemistry involved in the reaction to manufacture the substance, [redacted]

Therefore, [redacted] act as solvents and according to the substance definition in REACH, solvents which may be separated without affecting the stability of the substance or changing its composition should be excluded from the composition of the substance.

[2] https://echa.europa.eu/documents/10162/23036412/substance_id_en.pdf/ee696bad-49f6-4fec-b8b7-2c3706113c7d

You have stated that 2-methylpropan-1-ol cannot be separated without affecting the stability of the substance. However, the stabilising function has not been supported by any scientific evidence and it is confuted by the spectral data provided in IUCLID section 1.4. Indeed, the provided ^{13}C-NMR, ^{1}H-NMR and Infra Red spectra of the organic part of "sodium O-isobutyl dithiocarbonate" indicate that water and 2-methylpropan-1-ol are not present at a concentration level that is detectable by the spectral techniques used. These spectral data confirm that 2-methylpropan-1-ol and water can be removed without affecting the stability of the substance.

Therefore, without a stabilising function 2-methylpropan-1-ol (and water) must not be reported in the composition and must not contribute to the mass balance of the substance.

b. The substance is not a UVCB or multi-constituent substance because it has one main constituent

The SID Guidance clarifies in chapter 4.2. the following:

"*Substances of well defined chemical composition are named according to the main constituent(s).* […]

As a general rule, the aim should be to cover the composition up to 100%, and each constituent requires a complete chemical specification, including structural information. For substances that are defined by their chemical composition, a distinction is made between:

- *Main constituent: A constituent, not being an additive or impurity, in a substance that makes up a significant part of that substance and is therefore used in substance naming and detailed substance identification.*
- *Impurity: An unintended constituent present in a substance, as produced. It may originate from the starting materials or be the result of secondary or incomplete reactions during the production process. While impurities are present in the final substance, they were not intentionally added.*
- *Additive: A substance that has been intentionally added to stabilise the substance.*

All constituents (except additives) which are not the main constituent(s) in the mono-constituent substance or in the multi-constituent substance are considered to be impurities. […]

Some conventions are used to distinguish between mono-constituent and multi-constituent substances:

- *A mono-constituent substance is a substance in which one constituent is present at a concentration of at least 80% (w/w) and which contains up to 20% (w/w) of impurities.*
  A mono-constituent substance is named according to the one main constituent;
- *A multi-constituent substance is a substance consisting of several main constituents present at concentrations generally ≥ 10% and < 80% (w/w).*
  A multi-constituent substance is named as a reaction mass of two or more main constituents. […]"

A third type of substances according to the definition of the SID guidance are the substances of unknown or variable composition, complex reaction products or biological materials (UVCB substances). UVCB substances cannot be sufficiently identified by their chemical composition, because:

- The number of constituents is relatively large and/or
- The composition is, to a significant part, unknown and/or

- The variability of composition is relatively large or poorly predictable.

As a consequence, UVCB substances require other types of information for their identification, in addition to what is known about their chemical composition. In IUCLID dossier under section 1.2 for UVCB substances impurities are regarded as constituents all constituents and all the constituents are reported under the same composition block.

You have registered the substance selecting UVCB as substance type.

In IUCLID section 1.2, you have reported the followings as constituents:

- Sodium O-isobutyl dithiocarbonate, with typical concentration >[redacted]% (w/w) and concentration ranges [redacted]% (w/w);
- 2-methylpropan-1-ol, with typical concentration >[redacted]% (w/w) and concentration ranges [redacted]% (w/w); in the remarks field you have explained that 2-methylpropan-1-ol can not be separated without affecting the stability of the substance.
- Sodium hydroxide, with typical concentration <[redacted]% (w/w) and concentration ranges [redacted]% (w/w); in the remarks field you have explained that sodium hydroxide can not be separated without affecting the stability of the substance.
- Carbon disulphide, with typical concentration >[redacted]% (w/w) and concentration ranges [redacted] % (w/w);
- Disodium sulphide, with typical concentration >[redacted]% (w/w) and concentration ranges [redacted] % (w/w);
- Disodium carbonate, with typical concentration >[redacted]% (w/w) and concentration ranges [redacted] % (w/w);
- Water, with typical concentration <[redacted]% (w/w) and concentration ranges [redacted]% (w/w);
- Unknown or Minor constituents, with typical concentration <[redacted] % (w/w) and concentration ranges [redacted] % (w/w);

In IUCLID section 1.4 you have reported the following analytical data:

- ^{13}C-NMR, ^{1}H-NMR and Infra Red (IR) spectra of sodium O-isobutyl dithiocarbonate
- ^{13}C-NMR, ^{1}H-NMR and Infra Red (IR) spectra of 2-methylpropan-1-ol
- IR spectrum of sodium hydroxide.

However, the identification of the substance in your dossier does not follow the principles set out in the SID Guidance. Based on all the information you have provided, the identity and composition of the substance is known and the composition of the substance has a limited variability. Therefore, the substance is not a UVCB substance, but a well-defined substance and more specifically a mono-constituent substance.

Firstly, as explained in section 1.a., 2-methylpropan-1-ol and water are solvents which may be separated without affecting the stability of the substance or changing its composition must be removed from the mass balance.

Secondly, following the SID guidance, impurities are defined as all the unintentional constituents coming from the manufacturing process or from the starting material(s). These could be the result of secondary or incomplete reactions occurring during the production and are present in the final substance even if not sought by the manufacturer. According to the manufacturing process description provided in the dossier, [redacted]

[redacted]

Based on the above, it results that after moving the constituents described above to the impurity section, this substance contains only one main constituent "sodium O-isobutyl dithiocarbonate" (EC 246-805-2, CAS 25306-75-6, C5H10OS2.Na) present in a concentration well above 80% (w/w). This fact qualifies the substance as a mono-constituent substance.

The mono-constituent substance type is also confirmed by the analytical data provided in IUCLID section 1.4: the provided ^{13}C-NMR, ^{1}H-NMR and Infra Red spectra indicate that the organic part of the main constituent "sodium O-isobutyl dithiocarbonate" is present at a high purity level.
In addition, "sodium O-isobutyl dithiocarbonate" (EC 246-805-2, CAS 25306-75-6, C5H10OS2.Na) is already registered under the REACH Regulation as a mono-constituent substance.

In order to address the incompliance described above, you are requested to align the identification of the substance to the principles described in the SID guidance and in REACH:

- by identifying the substance as a mono-constituent substance type in IUCLID section 1.1.
- by reporting the main constituent "sodium O-isobutyl dithiocarbonate" (EC 246-805-2, CAS 25306-75-6, C5H10OS2.Na) as the main constituent of the substance.
- by reporting sodium hydroxide, carbon disulphide, disodium sulphide, and disodium carbonate under the impurity section in IUCLID section 1.2.

Under Article 3(1) of the REACH regulation, you are also requested to report for the substance in IUCLID section 1.2 only the amount of solvent(s) which cannot be removed without affecting the stability of the substance. For any quantity of solvents which cannot be removed, you must include evidence (for example in IUCLID section 1.4) to prove that such amount of solvent is necessary to guarantee the stability of the subtance. In such a case, the stabiliser solvent shall be included as an additive indicating the stabiliser function and shall not be contribute to the naming of the substance.
Finally, the main constituent, impurities and additives shall be reported with their typical concentrations and concentration ranges. The composition needs to be reported up to 100% of the substance. The composition of the substance must be supported by the analytical data provided in section 1.4.

You shall revise the identity in IUCLID section 1.1. by indicating that the substance is a mono-constituent substance and report the revised composition in IUCLID section 1.2.

Further technical details on how to report the information in IUCLID6 can be found in the manual "How to prepare registration and PPORD dossiers" available on ECHA website at the following link:
https://echa.europa.eu/documents/10162/22308542/manual_regis_and_ppord_en.pdf

In the comments to the draft decision you agree with the request.

Please note that this decision does not take into account updates of the registration dossiers after the date on which you were notified of the draft decision according to Article 50(1) of REACH (see section 5.4. of ECHA's Practical Guide "How to act in Dossier Evaluation").

2. Name or other identifier of the substance (Annex VI, Section 2.1.)

The name and other identifiers, required under Annex VI, Section 2.1, are used to identify the substance in an unambiguous manner and are therefore essential parts of substance identification. The information requirements listed in Annex VI, section 2.1. include: a name in the IUPAC nomenclature (section 2.1.1.), EINECS or ELINCS number (if available and appropriate) (section 2.1.3), CAS name and CAS number (if available) (section 2.1.4).

Specific requirements relating to mono-constituent substances, multi-constituent substances and UVCB substances are described in the SID guidance. Under these requirements, well-defined mono-constituent substances are named after the main constituent, using its IUPAC name. Other internationally recognized designations may be given as additional information. Instead, multi-constituent substances are named using the format "Reaction mass of [main constituents]", whereas UVCB substances are usually named "Reaction products of [starting materials]".

For the identification of the substance you have used the IUPAC name "Reaction mass of 2-methylpropan-1-ol and sodium O-isobutyl dithiocarbonate and sodium hydroxide" which is the format used for a multi-constituent substance.

However, as explained above under section 1, the available information in the dossier indicates that after the removal of the residual solvents from the composition and the requalification of impurities, this substance results in the substance being a substance with a single main constituent having a concentration >80% (w/w). According to the SID guidance, a well-defined substance with a single main constituent is a mono-constituent substance, which is named after the main constituent.

Moreover, even in case 2-methylpropan-1-ol could not be totally removed, but proved to be a stabilising additive (as clarified above in section 1) it would not contribute to the naming of the substance as explained in the SID guidance.

Therefore, in order to address this incompliance, you are requested to align the identification (name and numerical identifiers) of the substance with the correct composition and the analytical information by naming the substance after the main constituent "sodium O-isobutyl dithiocarbonate", which corresponds to the numerical identifiers EC 246-805-2 and CAS 25306-75-6.

In the updated dossier, the following actions must be done:

- Provide the chemical name "sodium O-isobutyl dithiocarbonate" in the "IUPAC name" field in IUCLID section 1.1.

- Do not remove or modify the current LIST entry 904-290-8 (this entry cannot be removed at this stage as this registration is linked to the current LIST entry in REACH-IT), but indicate in the "Remarks" field of the reference substance in IUCLID section 1.1, the following: "The list number 904-290-8 currently assigned does not specifically correspond to the substance. This identifier cannot be modified or deleted at this stage in the present registration update for technical reasons".

- Provide the CAS entry 25306-75-6 in the "CAS information" header of the reference substance in IUCLID section 1.1.

You should note that ECHA has established a process, subject to certain conditions, that enables registrants to adapt the EC identifier of an existing registration, while maintaining the regulatory rights already conferred to the substance concerned.

Pending the resolution of the non-compliances addressed in the present decision, any possible adaptation of the identifier can only become effective once ECHA is in a position to establish unambiguously the identity of the substance intended to be covered by you with this registration.
ECHA will inform you in due time as to when and how the identifier adaptation process must be initiated.

In any case, you should note that the application of the process of adapting the identifier does not affect your obligation to fulfil the requirements specified in this decision.

In the comments to the draft decision you agree with the request.

Please note that this decision does not take into account updates of the registration dossiers after the date on which you were notified of the draft decision according to Article 50(1) of REACH (see section 5.4. of ECHA's Practical Guide "How to act in Dossier Evaluation").

Appendix B. Procedural history

This decision does not prevent ECHA from initiating further compliance checks at a later stage.

ECHA followed the procedure detailed in Articles 50 and 51 of REACH

The compliance check was initiated on 25 June 2020.

ECHA notified you of the draft decision and invited you to provide comments.

ECHA took into account your comments and did not amend the request(s).

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 C. Addressee of this decision

Registrant Name	Registration number
[redacted]	[redacted]

Where applicable, the name of a third party representative (TPR) may be displayed in the list of recipients whereas ECHA will send the decision to the actual registrant