ECHA
EUROPEAN CHEMICALS AGENCY

GUIDANCE

Guidance for identification and naming of substances under REACH and CLP

September 2016
Draft Version 2.0

NOTE

Please note that the present document is a proposed new appendix to the *Guidance for identification and naming of substances under REACH and CLP*.

This document was prepared by the ECHA Secretariat for the purpose of this consultation and includes only the parts open for the current consultation, i.e. the above mentioned new appendix.

The full guidance document (version before proposed amendments) is available on the ECHA website at:

http://echa.europa.eu/guidance-documents/guidance-on-reach (version 1.4 published in June 2016).

After conclusion of the consultation and before final publication the new appendix will be included in the full document.

LEGAL NOTICE

This document aims to assist users in complying with their obligations under the REACH and CLP regulations. However, users are reminded that the text of the REACH and CLP Regulations is the only authentic legal reference and that the information in this document does not constitute legal advice. Usage of the information remains under the sole responsibility of the user. The European Chemicals Agency does not accept any liability with regard to the use that may be made of the information contained in this document.

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Appendix III

Reference: ECHA-xx-x-xx-EN
ISBN: xxx-xx-xxx-xxx-x
Publ.date: xxxx 2016
Language: EN

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Appendix III - Substance identification and joint submission of data

The core part of this guidance outlines the general principles potential registrants need to follow when identifying their legal entity specific substances to be registered. This Appendix gives practical guidance to potential registrants on how to apply substance identification principles when collectively defining the identity and scope of the substance identity for joint registration following the "One Substance - One Registration" (OSOR) principle of REACH. More information on the joint submission obligations and the data-sharing process in general is provided in the *Guidance on data-sharing* available at http://echa.europa.eu/guidance-documents/guidance-on-reach.
It is implicit that the same principles of substance identification given in the core guidance are applicable, according to the substance type, for the one substance identity for joint registration.

Indeed, the first parts of Article 11(1) and 19(1) of the REACH Regulation impose a requirement for "*joint submission of data by multiple registrants".* More specifically, these provisions require that "*when a substance is intended to be manufactured in the Community by one or more manufacturers and/or imported by one or more importers*" the information relating to properties of the substance and its classification "*shall first be submitted by the one registrant acting with the agreement of the other assenting registrant(s) (hereinafter referred to as "the lead registrant")*".

The Commission Implementing Regulation (EU) 2016/9 on joint submission of data and data-sharing reaffirms and consolidates the obligation of the multiple registrants of the same substance identity to submit certain information jointly. Practically, the joint submission of information requires the parties concerned to agree on the boundaries and scope of the substance identity. This is known as the substance identity profile or SIP. The jointly submitted Annex VII to Annex XI data is relevant for the full extent of the substance as described in the SIP.

Thus, the agreement on the scope of the substance identity covered by the registration is a pre-requisite to the joint submission. Transparency on the scope of this one substance identity and on the data to which it refers is central to implementation. Consequently, the scope of the substance or SIP must be reported in clear terms in the lead registrant's dossier on behalf of all the other registrants, while all registrants report their compositional information individually.

A simple illustrative example of a way to establish the substance identity profile for chemicals manufactured/imported in the EU by individual registrants is given schematically in Figure 1 below. It illustrates identifying the substance to be registered, aggregating the different compositions, generating the data and ultimately submitting it in IUCLID format in a registration dossier. The example is for a simple well-defined mono-constituent phase-in substance. For more complex substances, the process of defining the SIP may involve iterations between the figure's steps 3 and 5.

During the discussions among potential registrants, the SIP documentation can have the form of, e.g., a Word document or an Excel sheet where the relevant agreed information is recorded and made available to all members and potential members. Some industry

associations have made templates available for documenting the SIP and these have been used by many registrants (e.g. the Cefic template[1]). Others have simply documented the relevant information in a Word document or on the webpage of a consortium established to work on the registration of the substance concerned.

2. Defining the identity and scope of a substance corresponding to data submitted jointly

The steps that may be taken by multiple potential registrants in defining the substance identity corresponding to the data that they submit jointly are illustrated schematically in the example given in Figure 1 (steps 1 to 4) for simple well-defined substances.

Each individual potential registrant determines his obligations for what he manufactures/imports based on the definition of substance in Article 3(1) and applying the substance identification principles in the core part of this Guidance (steps 1 and 2 of Figure 1).

Each potential registrant can then check whether other potential registrants have reached the same "name & other identifiers" (step 3). From this starting point the potential registrants can collectively apply the principles of the core part of this guidance to define the boundaries of the substance identity corresponding to the data that they submit jointly; i.e. the substance identity profile (step 4).
This SIP describes in a generic manner the scope of the substance in terms of its compositional information (including any other relevant parameters such as morphology, e.g. physical form, shape), its name and other identifiers for which the classification and hazard data jointly submitted will be relevant. The definition of the SIP should not take an overly conservative approach to avoid excluding competitors from the joint submission.
This SIP establishes the inherent link between the substance identity and the hazard data to be jointly submitted. If established early enough, it can facilitate the stage of information generation/collection during the process of fulfilling registration obligations (outlined in the *Guidance on Information Requirements and Chemical Safety Assessment*; step 5 of Figure 1 below) in order to ensure that the data generated or collected covers the full extent of the substance identity.

As outlined in the core guidance sections 4.2.3 and 4.3, for more complex substances, additional parameters and/or descriptors for compositional information (e.g. description of the source/process) are normally used by potential registrants in steps 1-3 and those agreed can then be included in the SIP (step 4). In some cases, the link between the boundary of the substance identity and the hazard data jointly submitted may even become fully clear only when part or all of the available hazard data has been collected. There may be iterations between steps 3 - 5 as needed depending on the complexity of the substance identity and the data collected in step 5, e.g. when certain compositions include constituents that trigger classification and labelling and/or PBT assessment.

The SIP must provide generic information enabling the determination of the boundaries of the substance identity corresponding to the data jointly submitted:

[1] The Sip was originally described in Cefic "Guidance for Lead Registrants" available at http://www.cefic.org/Industry-support/Implementing-reach/Guidances-and-Tools1/. Examples of SIPs developed by registrants using this template can be found e.g. on the REACH centrum website http://www.reachcentrum.eu/consortium.html.

- name of the substance
- other identifiers (e.g. CAS, EC, molecular and structural information, description as relevant) covered by all the multiple registrants of the substance identity concerned
- compositional information:
  - identities of the constituents relevant for the substance identification and respective concentration ranges,
  - generic list of the identities of stabilizers relevant for the substance identification (and respective concentration ranges when applicable),
  - generic list of the additional parameters as relevant for the substance type (e.g. source process descriptors for some UVCBs)

It is important that the parameters defining the boundaries of the substance identity covered by the joint submission are agreed by all the joint registrants and are clearly documented in the SIP. Accordingly, a SIP may need to be modified or extended following the request of any new potential registrant, if they agree that part or all of the data jointly submitted is also relevant for the substance manufactured or imported by this registrant.

The SIP must not result in the sharing of confidential business information between registrants or the disclosure of such information to third parties from the joint submission. Where potentially confidential business information would need to be shared by the joint registrants in order to clearly define the SIP, they can consider using a trustee, as outlined in the *Guidance on data-sharing*.

In addition, a registrant can refuse that the SIP specifies an information specific to him and that he considers confidential business information (e.g. the presence of an impurity or an additive in the substances he manufactures or imports). In that case, the registrant shall nevertheless be liable for ensuring that his dossier takes full account of this information in order to preclude an underestimation of the hazards and risks of the substance. Firstly, the registrant shall specify explicitly and transparently the specific information in Section 1.2*)* of the IUCLID dossier. Secondly, for each endpoint that may be affected by the specific feature of the substance (e.g. impurity or additive), the registrant shall submit a scientific justification demonstrating the relevance of the data jointly submitted or submit the summary of a test performed on the substance comprising this feature. This information can be submitted separately in accordance with Article 11(3) or 19(2) of the REACH Regulation (so-called, 'opt out').

3. Practical guidance on documenting the substance identity profile

The general principles of substance identification for well defined and UVCB substances are outlined in the core guidance. Here below is some practical guidance on how to apply these principles collectively. The core guidance foresees that derogations from general principles are possible. Such derogations require the registrants to be able to demonstrate the inherent link between the substance identity and the hazard data jointly submitted.

3.1 Well-defined substances

For a well-defined substance, the >=80 % (w/w) principle for mono-constituent substance identification and the <80%, >= 10% principle for multi-constituent substance identification need to be followed when defining main constituent(s) and their concentration ranges and impurities. This applies to each individual registrant and to all multiple registrants collectively when determining the SIP. In particular, the impurity

profiles agreed in the SIP would need to be reported. Where the SIP includes specific impurities that would impact classification and labelling and/or PBT assessment, the registrants concerned by these impurities would need to consider these in the data gathering stage (step 5). The relevant Annex VII-XI information can be submitted jointly or submitted by them separately in accordance with article 11(3) of the REACH Regulation (so-called opt out options). The concentration values to be reported should take into account the concentration range across the joint submission.

For substances that require additional parameters to record the substance identification unequivocally, each registrant would need to follow the principles outlined in chapter 4.2.3 of the core part of this guidance. It should be considered whether variability in these parameters would trigger an adaptation, if necessary, of the classification or the hazard data jointly submitted. For the purpose of determining the SIP in relation to joint submission, similar considerations may be applied. For example, it may be necessary to include in the substance identity profile those parameters (e.g. physical form and/or morphological parameters like porosity, particle size, particle shape) which may impact properties relevant for determining the hazard profile (e.g. solubility, reactivity, inhalation toxicity, etc.). Where this is the case, the generic ranges of these parameters covered by the SIP would need to be provided transparently (e.g. particle size ranges applicable to all registrants and list of their shape(s) and list of surface chemistries). Thus, the comprehensiveness of the hazard data jointly submitted in relation to the SIP is ensured.

Similarly, differences in the crystalline phase of inorganic chemicals may trigger different hazard profile considerations specific to these phases (e.g. quartz, cristabolite, amorphous silica). Taking account of the possible difference in the properties of the various phases, it is for the potential registrants of these substances to consider whether to submit one joint registration covering all the phases, including hazard data specific to different phases, or to submit different joint registrations for different phases (i.e. different substance identities). In either case, the phases covered would need to be listed in the SIP and the relevant Annex VII-XI data would need to address all phases covered by the registration, thus ensuring that the data covers the full extent of the SIP.

3.2 UVCB substances

For UVCBs, the identification can be more challenging and for this reason transparent documentation is very helpful in agreeing on the substance identity for the joint registration. Each potential registrant would need to consider the advice in the core part of this guidance individually and then apply the same principles collectively. Note the aggregation of concentration ranges into the SIP could lead to a profile with very broad concentration ranges, possibly up to a point that it cannot be considered as one substance anymore.

As outlined in the core guidance, the basis for the identification of some UVCB substances is the source and process used in their manufacture rather than directly the identities and concentration ranges of their constituents. In these cases, other descriptors serve as proxies for the constituent identities and their respective concentration ranges. Potential registrants may describe the manufacturing process in terms of source and process to the extent necessary to identify the substance. The description may include any additional parameters/characterizers that registrants decide are relevant for their substance identity (see for example table 4.2 in the core guidance). For the purpose of the joint registration, the descriptions are shared solely as needed to agree the scope of the UVCB substance identity for registration. Potential registrants can follow the principles outlined in the core guidance both individually and then collectively. The SIP thus results in generic reporting of the source and process parameters so that it

covers the full extent of the compositions of the individual registrants. This is illustrated schematically in Figure 2.

For substances identified based on source and process, as outlined in the core guidance any significant change of source or process would be likely to lead to a different substance identity that should be registered separately. Derogations from this principle would mean that the registrants can demonstrate that each process/source combination yields compositions that can be addressed in the same joint registration. Minor variations in source materials and process and/or process conditions can be taken into account in the SIP. Registrants should agree that each process/source combination yields compositions that are similar to the extent that it is meaningful to cover them as one substance identity and make sure that the hazard data is appropriate for the whole area of variation of the SIP. More specifically, the registrants must be able to justify that the hazard data set jointly submitted is relevant for all these compositions or is adapted, where relevant, with information submitted separately for specific compositions under Article 11(3) of REACH (opt out).

In order to demonstrate the relevance of the data set for each process/source combination, these combinations need to be transparently documented in the SIP to document inclusion/exclusion criteria applied for current and future joint registrants.

For other types of UVCB (see chapter 4.3.2 of the core guidance), a combination of compositional and additional descriptors may be used by the potential registrants as relevant. For instance, for some oleochemicals, the composition is variable due to variability in the alkyl chain length distributions of the constituents and the alkyl chain length distribution can be an additional descriptor used in identification. The approach taken by the SIEF would need to be documented transparently in their SIP.

3.3 Substance identity profile

It is the responsibility of all registrants submitting information jointly to agree on the necessary parameters for their substance identification and document them transparently in their corresponding SIP. Deviations or derogations from normal substance identity principles taken collectively would need to be transparently documented. As the SIP documents the inclusion/exclusion criteria, the SIEF would need to ensure that the criteria applied are transparent and that the relevant Annex VII-XI data collected/generated demonstrably covers all compositional profile(s) agreed.

Where potential registrants individually include stabilizing additives in the context of Article 3(1) in their identity profile, their identities and concentration ranges need to be agreed and transparently reported in the SIP.

In the data gathering stage, the relevance of the test material(s) used to generate/collect data to fulfil Annex VII-XI information requirements would need to be considered. The rationale for conclusions on their representativeness for the compositions covered by the SIP would need to be documented and included in the technical dossier. This would in particular be relevant for complex substance identities that cover broad compositional profiles.

The potential registrants may determine during the data gathering that their SIP is overly broad and it is not fit for the purpose of submitting jointly hazard information that

is representative of the substance identity concerned. In such a case, the potential registrants may decide to split the SIEF to address separately two or more substances[2]. Each substance would then have its own SIP and its own joint submission of hazard information that must be specifically representative for that substance identity. The reasons why certain hazard information was not representative for certain parameters of the substance identity would need to be transparently documented in the SIP for each separate registration. The respective potential registrants may also determine at this stage that the compositional profiles need to be further refined based on constituents and/or impurities triggering classification and labelling, PBT assessment, etc.

For potential registrants intending to join other potential registrants where a SIP has already been agreed by them and the registration has not yet been submitted, they would need to consider whether their substance identity information is within the boundaries of the SIP. Where it is not, they would need to discuss and agree with potential registrants whether it is necessary either to expand the scope of the profile to include the new member or to agree that it is not within scope.
An adaptation of the SIP would be required if the substance to be registered by the potential registrant has specific substance identity parameters that may alter the representativeness of the hazard information jointly submitted and therefore require a specific justification (e.g. a specific impurity, a different composition ratio, a different phase, a different particle size, etc.). For the sake of transparency, this parameter will have to be specified in the SIP.
Alternatively, the potential and existing registrants may agree that the hazard data jointly submitted is fundamentally not representative for the substance of the potential registrant. In that case, the potential registrant shall submit a separate registration either together with other registrants with a substance identity comprising this parameter, or individually if there would be no other registrants for the same substance identity.

4. Reporting the substance identity profile in the registration dossier

When the potential registrants have collected/generated all required Annex VII-XI data for their substance (i.e. step 5 in Figure 1), the data package is ready to be reported in IUCLID format in dossiers for submission to the Agency (i.e. step 6 in Figure 1). To report the SIP in IUCLID format, the name and other identifiers, the compositional information and other parameters as relevant are reported in IUCLID sections 1.1 and 1.2.

Substance identity profile	Reported in IUCLID
name and other identifiers	Section 1.1 of all dossiers
compositional information and other parameters as relevant	Section 1.2 of the lead registrant dossier

The SIP name and other identifiers are reported in section 1.1 of all dossiers. The lead registrant reports the SIP compositional information and other parameters as relevant in

[2] Considerations on the role of EINECS in establishing substance identity under REACH can be found in the CARACAL paper agreed at the 4th Meeting of the Competent Authorities for REACH and CLP (CARACAL): CA/74/2009 rev.2 "Substance identity and SIEF formation (the role of EINECS)".

section 1.2 of his dossier in the form of a "boundary composition of the substance"[3]. The lead registrant must also submit all relevant Annex VII-XI data in sections 4-14 (in the absence of justified opt-outs for one or more information requirements) on behalf of all registrants.

Each registrant (including the lead registrant) reports his own legal entity compositional information of the substance he specifically manufacture or import in section 1.2 of his own dossier. This means that the lead registrant reports both the SIP compositional information and his own legal entity compositional information in section 1.2 of his dossier while all other registrants report their own specific compositional information. Each standard registration must also include the relevant analytical information in section 1.4 of IUCLID.

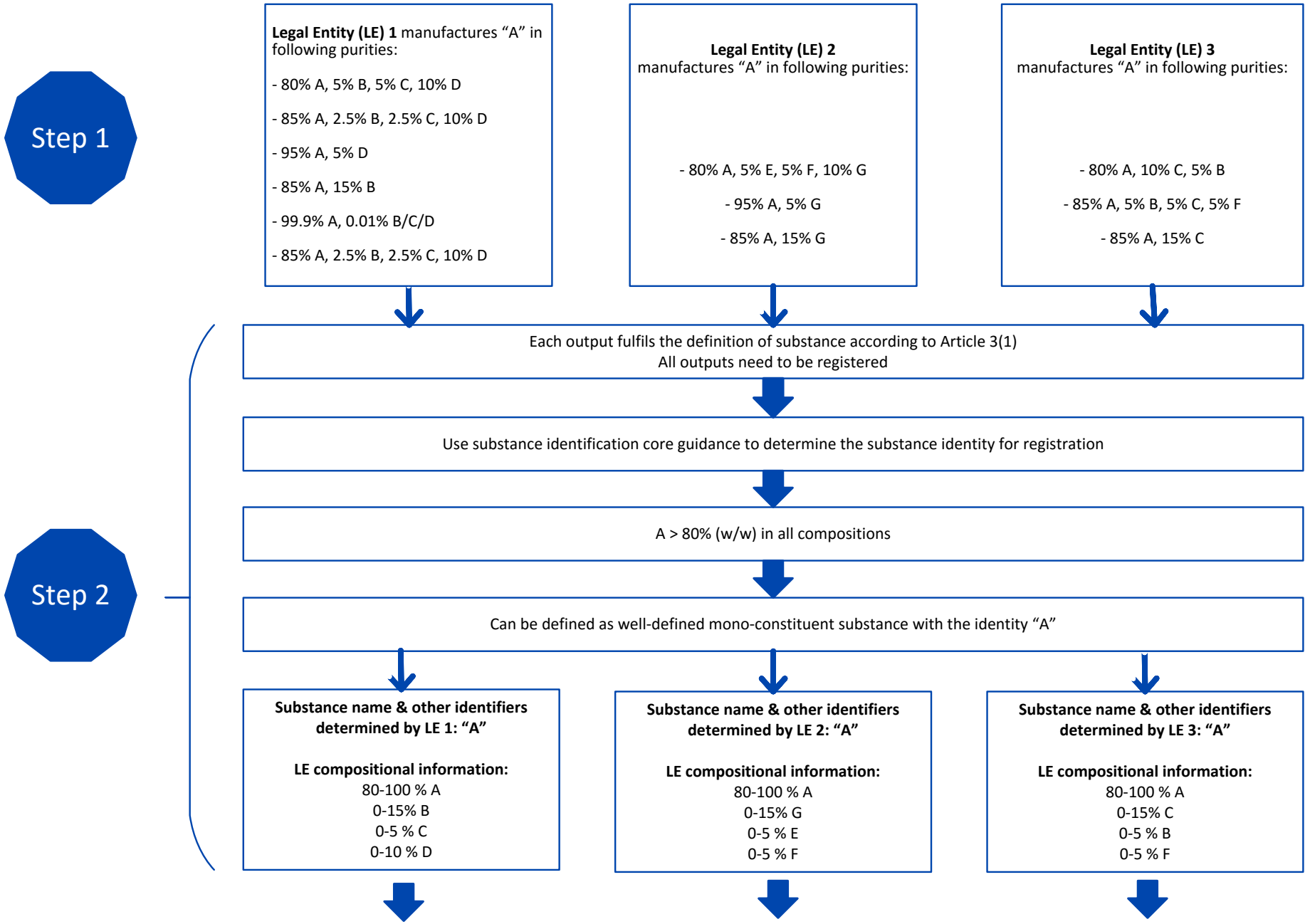
Each registrant should demonstrate that the compositional information of the substances he specifically manufactures or imports is covered by the SIP as reported in the "boundary composition" and in turn is covered by the Annex VII-XI data submitted in the lead registrant dossier (in the absence of justified opt-outs).

Technical instructions on how to report compositional information in IUCLID format is available in the IUCLID manuals (http://echa.europa.eu/manuals).

5. Transition measures between IUCLID 5 and 6

Fields were not available in IUCLID 5 to transparently report the SIP compositional information in section 1.2 in the lead registrant dossier. Some lead registrants had been providing this information using labels to indicate that the information referred to the SIP.
IUCLID 6 supports this reporting in a systematic transparent manner. Technical details are available in the relevant IUCLID manual.
The document "Transition to the new IT tools – how to prepare" (available at http://echa.europa.eu/manuals) provides details on transition measures for lead registration dossiers submitted in IUCLID 5 that submit updates in IUCLID 6 and are required to include the substance identity compositional information in section 1.2 are available on the ECHA website.

[3] Instructions how to enter the "boundary composition of the substance" can be found in the manual "How to prepare registration and PPORD dossiers" available at http://echa.europa.eu/manuals.


Step 1
Legal Entity (LE) 1 manufactures "A" in following purities:
- 80% A, 5% B, 5% C, 10% D
- 85% A, 2.5% B, 2.5% C, 10% D
- 95% A, 5% D
- 85% A, 15% B
- 99.9% A, 0.01% B/C/D
- 85% A, 2.5% B, 2.5% C, 10% D
Legal Entity (LE) 2 manufactures "A" in following purities:
- 80% A, 5% E, 5% F, 10% G
- 95% A, 5% G
- 85% A, 15% G
Legal Entity (LE) 3 manufactures "A" in following purities:
- 80% A, 10% C, 5% B
- 85% A, 5% B, 5% C, 5% F
- 85% A, 15% C
Step 2
Each output fulfils the definition of substance according to Article 3(1)
All outputs need to be registered
Use substance identification core guidance to determine the substance identity for registration
A > 80% (w/w) in all compositions
Can be defined as well-defined mono-constituent substance with the identity "A"
Substance name & other identifiers determined by LE 1: "A"
LE compositional information:
80-100 % A
0-15% B
0-5 % C
0-10 % D
Substance name & other identifiers determined by LE 2: "A"
LE compositional information:
80-100 % A
0-15% G
0-5 % E
0-5 % F
Substance name & other identifiers determined by LE 3: "A"
LE compositional information:
80-100 % A
0-15% C
0-5 % B
0-5 % F

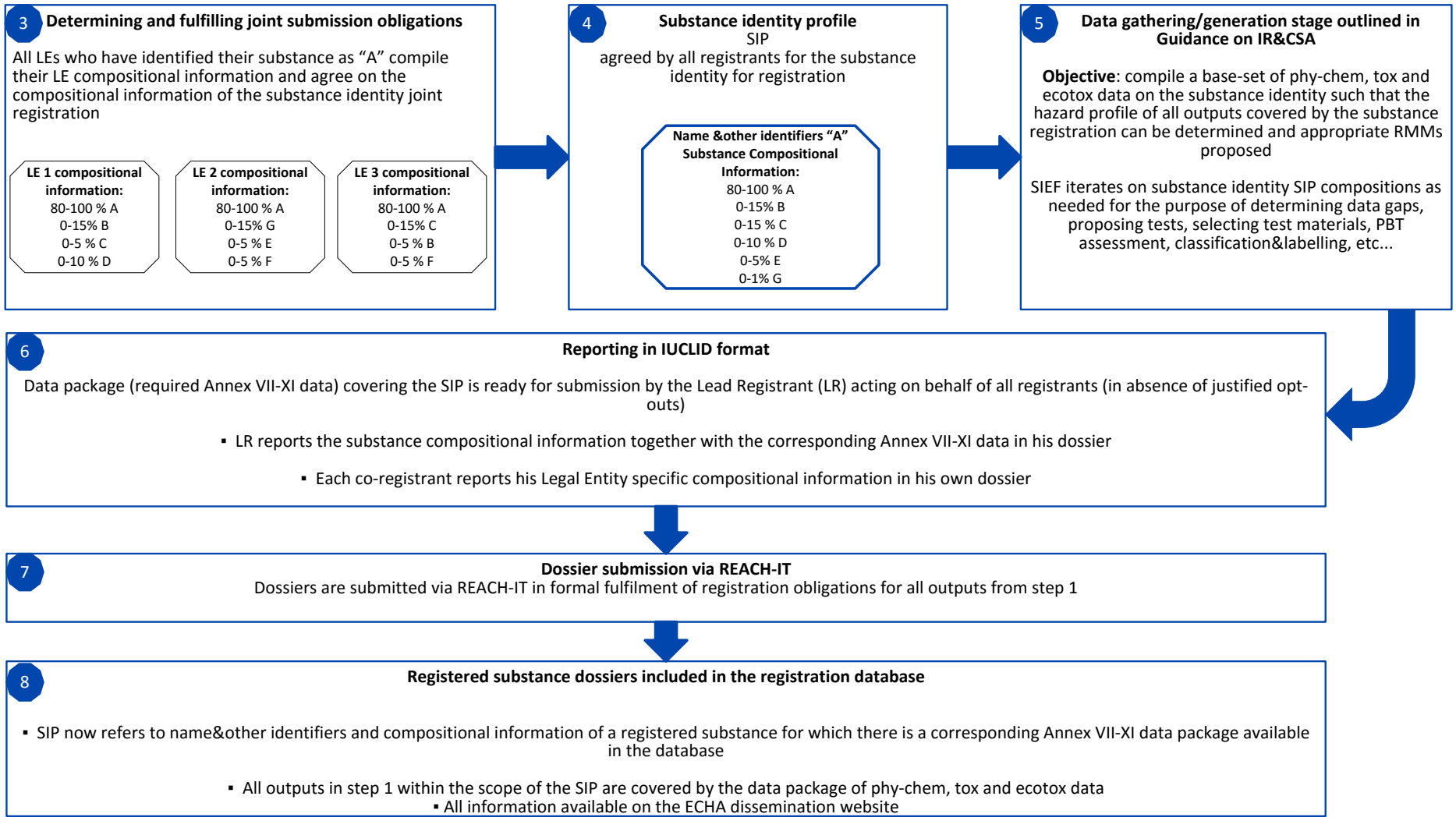


Figure 1 a schematic overview of the steps potential registrants take from determining their registration obligations (1) to defining their SIP for their one substance identity (4) and ultimately submitting their registrations in formal fulfilment of the obligations to register their substances (8). The substance identity is a simple mono-constituent to make it simpler to visualise. For more complex substances, the steps are the same but additional elements and/or proxies for compositional information may be used to define substance identity. The process of defining the SIP may also involve iterations between steps 3 and 5.

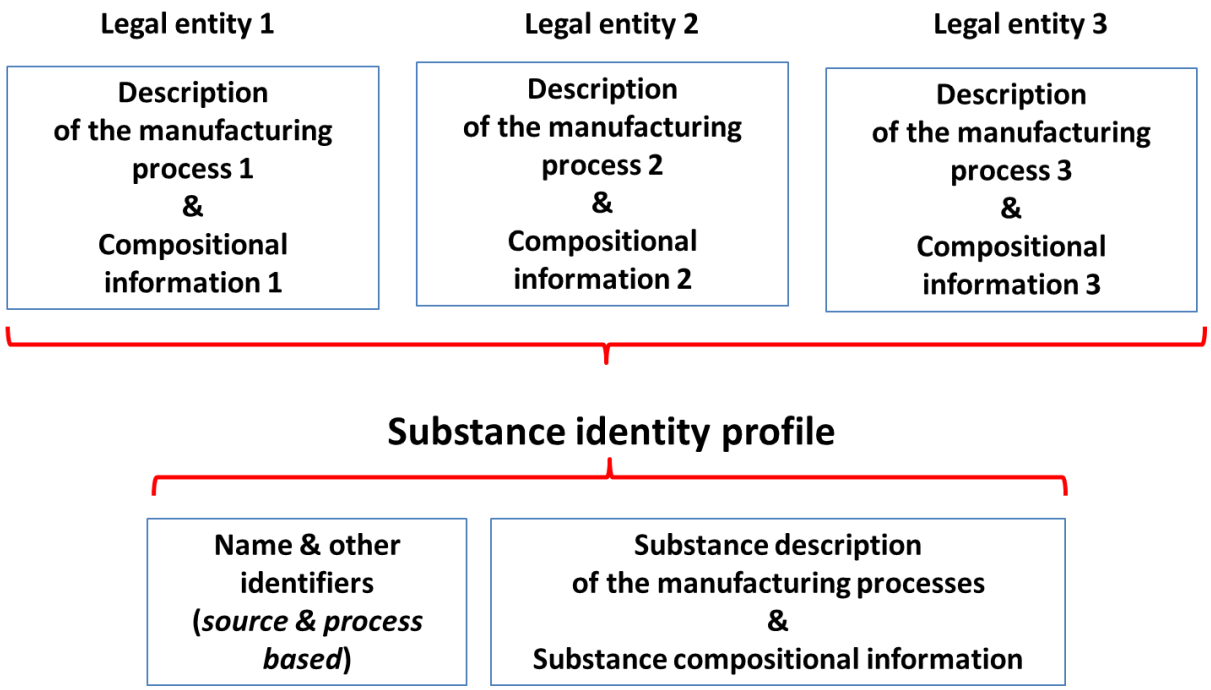


Figure 2. Illustrative schematic of defining a SIP (step 4 in Figure 1) for a UVCB type substance identified based on source and process descriptors from individual legal entity source & process descriptions.

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