

Technical instructions on how to report substance identity information for CICPs in IUCLID 6

The instructions below aim to guide potential Registrants and existing Registrants on the reporting of substance identity data in IUCLID 6, when preparing or updating registration dossiers for complex inorganic coloured pigments (CICPs). The instructions provide guidelines on the reporting of substance identity information that is particular for CICPs and at the same time provide tips to avoid failing the completeness check when submitting a dossier.

However, before submitting the dossier, the Registrant should use the IUCLID Validation Assistant both on the substance dataset and on the final dossier to check if any completeness failures are detected.

It should also be noted that, passing the checks of the Validation Assistant does not automatically mean that the dossier is complete. The dossier will be subject to a manual check when submitted and if issues are found in the dossier during the manual check, the Registrant will receive a letter from ECHA with instructions on how to make the dossier complete.

Instructions on the reporting substance identity of CICPs in IUCLID 6 (section 1.1 and 1.2)

To report identity of your CICPs in IUCLID 6, please follow the instruction provided in section 9.4 of the manual "*How to prepare registration and PPORD dossiers*" (version 4.0, May 2017) (hereafter "the manual") available in the ECHA website¹ in combination with the specific instruction provided in this document.

Below are listed the sections and steps of the manual where specific instructions are necessary for the reporting of CICPs:

Section 9.4. Section 1 General information

9.4.1. Section 1.1 Identification

Step 7:

Create a new reference substance (instruction on how to create a new reference substance are in section 6.1 of the manual)

- 1) IUPAC name: follow the nomenclature principles outlined in the "Guidance document for the Registration of Complex Inorganic Coloured Pigments".
- 2) Molecular formula representing all compositions covered by the joint submission: report the stoichiometric variability of the CICPs within the joint submission.

¹ https://echa.europa.eu/documents/10162/22308542/manual_regis_and_ppord_en.pdf

EXAMPLE:

Joint registration covering CICPs with compositions with two different minor elements.

1

- Main elements (present $\geq 10\%$ expressed as oxides):

M1 (range of stoichiometric ratio: 1-1.5)

M2 (range of stoichiometric ratio: 0.9-1.1)

- Minor element (present $< 10\%$ expressed as oxides):

M3 (range of stoichiometric ratio: 0.05-0.08)

- Oxygen present in a stoichiometric ratio of 4

2

- Main elements (present $\geq 10\%$ expressed as oxides):

M1 (range of stoichiometric ratio: 1-1.2)

M2 (range of stoichiometric ratio: 0.8-1.5)

- Minor element (present $< 10\%$ expressed as oxides):

M4 (range of stoichiometric ratio: 0.03-0.04)

- Oxygen present in a stoichiometric ratio of 4

» The information in the molecular formula field can be reported as:

$M_1xM_2yM_3zM_4wO_4$ ($1 \leq x \leq 1.5$, $0.8 \leq y \leq 1.5$, $0 \leq z \leq 0.08$, $0 \leq w \leq 0.04$)

Step 8:

Substance type: UVCB

9.4.2. Section 1.2 Composition

Note: The lead registrant dossier should report two types of composition records (the legal entity specific composition record(s) and the boundary composition of the substance record(s)).

The member registrant dossier should report the specific legal entity composition record(s). It can also report the boundary composition record(s), but it is not mandatory.

General information:

Legal entity specific composition record(s)

Step 2:

Select "legal entity composition of the substance" for the "type of composition" field.

Step 4:

In the "Description" field report the description of the manufacturing process which is legal entity specific and provides details on the identity and ratio of starting materials, reaction type and any relevant parameter of the process (e.g, temperature, pressure).

e.g : *The pigment is the reaction product of high temperature calcination in which M1 oxide, M2 oxide and M3 oxide in a ratio of X:Y:Z are homogeneously and ionically interdiffused at x°C and x Pa to form a crystalline matrix of xxxxx.*

Step 6:

In the "Justification for deviations" field provide the justification for having only one constituent reported (if applicable). The justification should justify the deviation of reporting the composition of a UVCB substance (expected to have a variable complex composition) with only one constituent.

One example of a valid justification would be:

"The substance is a UVCB due to variations at the elemental level and these variations cannot therefore be represented by reporting different constituents but only in the form of a variable molecular formula."

Step 9:

The substance identity is reported as UVCB, therefore as described in the "Guidance for identification and naming of substances under REACH and CLP" (version 2.1, May 2017), all constituents present in the composition of the substance are equally reported as constituents without distinguishing main constituents and impurities. If certain constituent is considered as an impurity, this can be indicated in the "Remarks" field of the constituent in question.

The unknown or variable minor constituents can be grouped in one reference substance called "unknown impurities" and the available information regarding the identity and content should be reported in the "Remarks" field.

Step 10:

Note: In case one legal entity covers more than one combination of minor elements, it is recommended to be created a composition record for each possible combination. This will provide a clear overview of the substance covered by the legal entity.

Create a new reference substance (instruction on how to create a new reference substance are in section 6.1 of the manual):

- 1) IUPAC name: Main and minor elements with crystalline structure (e.g. M1, M2, M3, M4, [crystal structure]).
- 2) Legal entity specific molecular formula: report the stoichiometric variability of the CICP.

EXAMPLE

CICP with

- Main elements (present $\geq 10\%$ expressed as oxides):

M1 (range of stoichiometric ratio: 1-1.5)

M2 (range of stoichiometric ratio: 0.9-1.1)

- Minor element (present $< 10\%$ expressed as oxides):

M3 (range of stoichiometric ratio: 0.05-0.08)

- Oxygen present in a stoichiometric ratio of 4

➤ The information in the molecular formula field can be reported as:

$M_1xM_2yM_3zO_4$ ($1 \leq x \leq 1.5$, $0.9 \leq y \leq 1.1$, $0.05 \leq z \leq 0.08$)

Assign the created reference substance to the constituent corresponding to the CICP. The "Remarks" field can be used to indicate which of the minor elements reported in the molecular formula are not included in the boundary composition (if any).

For the other constituents (usually considered as impurities in the CICPs sector) create (as necessary) and assign the appropriate reference substance.

Note: If you report only one constituent, you should provide a justification in the "Justification for deviations" field (see step 6 above).

Boundary composition record(s)

Note: The boundary composition record(s) is a technical reporting of the constituents and related concentration ranges covered by the joint submission and therefore, should ideally describe the crystal structure, the main elements, all possible minor elements covered and all possible impurities.

In case of large number of possible combinations of minor elements within a joint submission, ECHA recommends reporting a boundary composition record for each possible combination. This would provide a clear overview of what the substance identity of the joint submission consists of and might be useful to explain how the data submitted in Annex VII-XI covers the full extent of what has been registered. However, it is up to each joint submission to decide the best strategy to report the boundary composition.

When more than one boundary composition record is reported, it is recommended to use Assessment entities (see chapter 9.3 Assessment entity of the manual) to structure the information reported across the different IUCLID dossier sections. The assessment entity reporting tool in IUCLID 6 will facilitate registrants demonstrate the relevance of their hazard/fate data with the compositions registered. Note that where substance identity has been defined broadly, registrants will need to be able to demonstrate that their reported Annex VII-XI data covers the full extent of what has been registered by them in terms of test materials.

Step 1:

The descriptive name should describe the specific combination of metals (e.g. M1 M2 with M3 and M4 as minor elements).

Step 2:

Select “*boundary composition of the substance*” for the “*type of composition*” field.

Step 4:

In the “Description” field report a manufacturing process description that generically describes all the different manufacturing processes covering the specific combination of elements in the pigment.

e.g : The pigment is the reaction product of high temperature calcination (>XXX °C /XXX-XXX °C) in which raw materials M1,M2andM3 o(expressed as oxides) and possibly others are homogeneously and ionically interdiffused to form a crystalline matrix of xxxxx.

Step 6:

As for the Legal entity specific composition record.

Step 9:

As for the Legal entity specific composition record.

Step 10:

Create a new reference substance (instruction on how to create a new reference substance are in section 6.1 of the manual):

- 1) IUPAC name: Main and minor elements with crystalline structure (e.g. M1, M2, M3, M4, [crystal structure]).
- 2) Molecular formula representing the specific combination of elements: report the stoichiometric variability of the CICIP.

EXAMPLE:

Joint registration covering CICPs with compositions with two different minor elements.

Two boundary composition records can be created reporting the two different elements combination.

1

- Main elements (present $\geq 10\%$ expressed as oxides):

M1 (range of stoichiometric ratio: 1-1.5)

M2 (range of stoichiometric ratio: 0.9-1.1)

- Minor element (present $< 10\%$ expressed as oxides):

M3 (range of stoichiometric ratio: 0.05-0.08)

- Oxygen present in a stoichiometric ratio of 4

» The information in the molecular formula field for this elements combination can be reported as:

$M1xM2yM3zO4$ ($1 \leq x \leq 1.5$, $0.8 \leq y \leq 1.5$, $0.05 \leq z \leq 0.08$)

2

- Main elements (present $\geq 10\%$ expressed as oxides):

M1 (range of stoichiometric ratio: 1-1.2)

M2 (range of stoichiometric ratio: 0.8-1.5)

- Minor element (present $< 10\%$ expressed as oxides):

M4 (range of stoichiometric ratio: 0.03-0.04)

- Oxygen present in a stoichiometric ratio of 4

» The information in the molecular formula field for this elements combination can be reported as:

$M1xM2yM4wO4$ ($1 \leq x \leq 1.5$, $0.8 \leq y \leq 1.5$, $0.03 \leq w \leq 0.04$)

Assign the created reference substance to the constituent corresponding to the CIPC.

For the other constituents (usually considered as impurities in the CICPs sector) assign or create the appropriate reference substance.