Introduction to Substance Identification

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Outline

• Importance of the substance identification
• Substance identity requirements under REACH
• Basic principles of the substance identity
  o Key definitions
  o Identification of mono-constituent substances
  o Analytical information requirements
• Substance identity in IUCLID
Why is Substance Identification important?

- Defines the scope of the registration
  - To ensure that the substance identity is clearly defined for hazard and risk communication
  - To ensure that the registration covers one individual substance

- To ensure that the chemical identity of your substance is clear to ECHA
  - To establish whether two (or more) substances are the same

- To facilitate data sharing and joint submission
Legal references

Article 11(1) of the REACH Regulation:

- Each registrant shall submit separately information on substance identity as specified in Annex VI (2)
What is a substance?

- Article 3 of the REACH Regulation states:

  "**substance**: means a chemical element and its compounds in the natural state or obtained by any manufacturing process, **including** any additive necessary to preserve the stability and 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"
Substance identity requirements

• Annex VI (2) of the REACH Regulation states:

“For each substance, the information given in this section shall be sufficient to enable each substance to be identified. If it is not technically possible or if it is does not appear scientifically necessary to give information on one or more of the items below, the reasons shall be clearly stated”

• Main points of Annex VI (2):
  o 2.1 Name or other identifier of each substance
  o 2.2 Information related to molecular and structural formula of each substance
  o 2.3 Composition of each substance
## Substance identity requirements (Annex VI (2) of REACH)

<table>
<thead>
<tr>
<th>Section</th>
<th>Requirement</th>
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</thead>
<tbody>
<tr>
<td>2.1.1</td>
<td>IUPAC name or other international chemical name</td>
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<tr>
<td>2.1.2</td>
<td>Other names (e.g. trade name)</td>
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<td>2.1.3</td>
<td>EINECS or ELINCS number (if available)</td>
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<td>2.1.4</td>
<td>CAS name and CAS number (if available)</td>
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<td>2.1.5</td>
<td>Other identity code (if available)</td>
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<tr>
<td>2.2.1</td>
<td>Molecular and structural formula (including SMILES, if available)</td>
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<tr>
<td>2.2.2</td>
<td>Information on optical activity and typical ratio of (stereo) isomers (if applicable and appropriate)</td>
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<td>2.2.3</td>
<td>Molecular weight or molecular weight range</td>
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<tr>
<td>2.3.1</td>
<td>Degree of purity (%)</td>
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<tr>
<td>2.3.2</td>
<td>Nature of impurities, including isomers and by-products</td>
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<tr>
<td>2.3.3</td>
<td>Percentage of (significant) main impurities</td>
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<td>2.3.4</td>
<td>Nature and order of magnitude (e.g. ppm) of any additives (e.g. stabilising agents or inhibitors)</td>
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<td>2.3.5</td>
<td>Spectral data (ultra-violet, infra-red, nuclear magnetic resonance or mass spectrum)</td>
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<td>2.3.6</td>
<td>High-pressure liquid chromatogram, gas chromatogram</td>
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<td>2.3.7</td>
<td>Description of analytical methods or the appropriate bibliographical references for the identification of the substance and, where appropriate, for the identification of impurities and additives. This information shall be sufficient to allow the methods to be reproduced.</td>
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Basic principles of substance identity

A substance is, in general, identified by its name, chemical composition and numerical identifiers.

- **Well-defined substances**
  - Structure of the main constituent(s) is known
  - IUPAC name and other identifiers

- **Not well-defined substances (Unknown or Variable composition, Complex reaction products or Biological materials)**
  - Cannot be sufficiently identified by their composition
• Identification of the substance type: well-defined vs. UVCB

*From “Guidance for identification and naming of substances under REACH and CLP” available at ECHA webpage

http://echa.europa.eu
Well-defined substances – definitions:

**Main constituent**

- A constituent, not being an additive or impurity, in a substance that makes up a *significant part* of that substance
- Contributes to the *naming* of the substance
- Concentration of the main constituent(s) = purity of the substance
Well-defined substances – definitions (cont):

**Impurity**

- An unintended constituent present in a substance, as produced; **not intentionally added** (e.g. unreacted substrate)
- **Not included** in the substance name
- Identification and quantification required for all impurities (including isomers and by-products) \( \geq 1\% \) or relevant for the classification and/or PBT assessment (irrespective of their concentration)

**Additive**

- A substance that has been intentionally added to **stabilise** the substance
- Contributes to the substance composition (but not to the naming)
Mono-constituent substances

- Composition is **known** (exact structure, stoichiometry etc.)
- Concentration of the main constituent \(\geq 80\% \, (w/w)\)
- Up to **20\% \, (w/w)** of impurities
- Naming
  - Named after the **main constituent**
    - Usually according to the recent IUPAC nomenclature rules
    - In the English language
Mono-constituent substances (cont.)

• Identification
  - IUPAC name, EINECS or ELINCS number (if available and appropriate), CAS name and CAS number (if available), other identity name or code (if available), information related to molecular and structural formula
  - **Same** main identifiers for each joint registrant of the substance

• Composition
  - Purity (=concentration of main constituent), impurities and additives together with relevant identifiers and **concentrations** (typical and **ranges**)
  - Composition completed up to **100%**
  - Main constituent **same** for each registrant (concentration ranges may differ), impurities **specific** for each joint registrant
Analytical data

Qualitative analytical methods and results (identification)

- **UV/Vis** (190-800 nm), **IR** (400-4000 cm⁻¹), **¹H NMR** (0-15ppm)
- If necessary: **¹³C NMR**, **MS**, **XRD** and or more appropriate
- **All** (ionic) parts of the substance need to be determined
Analytical data (cont.)

Quantitative analytical methods and results (composition)

- Quantification of all constituents > 1%
- **GC** or **HPLC**
- If necessary other methods: AAS, ICP, XRF, QXRD, titration, GCxGC
- For ionic constituents, each ion should be quantified
- Direct quantification instead of back-calculations (e.g. 100%-sum of impurities **not acceptable**)

Description of analytical methods

• Annex VI (2.3.7): “The description should be given in such detail that the method can be reproduced.”

- **NMR** (integration, solvent used, NMR measurement parameters)
- **UV/Vis** (solvent, concentration, path length)
- **IR** (IR measurement parameters, sample preparation)
- **Chromatography** (detailed description of experimental set up, peak table, peaks assigned to constituents, details of calibration and calculations used)
- Other methods: XRF/XRD (Source, current, voltage, refinement method)
Substance identity in IUCLID 5
Substance identity in IUCLID 5

Substance identifiers

Identity and concentration of all constituents

Quantitative and qualitative analytical methods and results

All the information in these three sections must be consistent
Section 1.1 (cont.)

Check pre-filled fields and correct if necessary

Complete missing information

Make sure that all identifiers are consistent (IUPAC name, structural formula, EC number, CAS name and number, molecular formula and weight, SMILES notation etc.)
Identify (main) constituent(s), impurities and additives.

Provide IUPAC name and structural formula for each constituent.

EC number, CAS name and CAS number, SMILES notation etc. should be provided if available.

All manufactured and/or imported compositions should be reported.
IUCLID Section 1.2 (cont.)

Ensure that information in section 1.2 is consistent with analytical data provided in section 1.4

- Number of main constituents and their concentrations;
- Number of impurities and their concentrations;
- Degree of purity

Provide degree of purity for the substance

Provide typical, minimum and maximum concentrations for (main) constituents, impurities and additives
Attach the analytical information as required in Annex VI (2) of the REACH Regulation:
- UV, IR and NMR/MS spectra
- HPLC/GC
- description of the analytical methods

Make sure the results of the analysis are consistent with the information provided in section 1.2.

You need to include scientific justification for not providing information as required in Annex VI, section 2 of the REACH Regulation.

If the techniques mentioned in Annex VI (2) of the REACH Regulation are not suitable for your substance, please provide data from another characterisation method (e.g. for inorganic substances: XRD and elemental analysis)
Summary

- Substance identification is a **pre-requisite** to most of the REACH processes and must be clearly addressed

- **Each** joint registrant shall submit **separately** information on **substance identity** as specified in **Annex VI (2)** of REACH

- Information on substance identity shall be **consistently** reported in the IUCLID 5 dossier
Thank You
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