Substance identity - UVCB substances

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Unit C2 – Substance identification and data sharing

Aims of this presentation

- To highlight how elements of UVCB substance identity (SID) should be presented in the dossier

➢ ... by providing some practical advice

- To help lead registrants to understand why ECHA requires certain UVCB SID information

➢ ... and to what level of detail

What is a UVCB substance?

- Substance of Unknown or Variable composition, Complex reaction products or Biological materials

- Cannot be sufficiently identified by its 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

- If the chemical composition of, for example, a complex reaction product is known
  - ➢ Identification either as mono- or multi-constituent substance should be considered

Appropriateness of EC/CAS identifiers

- ✓ Only assign an EC/CAS identifier that fits to your substance
- ✓ Check carefully whether a certain EC/CAS number/name is specific to your substance
- ✓ Make sure it does not cover multiple substances
- ✓ In EINECS there are published descriptions which form part of the substance identity –where these entries are used you should check whether your substance fits to this description

IUPAC name for UVCB substances

- IUPAC rules cannot be easily applied to UVCB substances
- Consequently the term “IUPAC” is not so relevant
- However, a “substance” name should be provided
- The naming of UVCB substances is specific to the UVCB type
- Broadly addressed in the ECHA guidance on SID
- More detailed guidance on naming of specific types of UVCB substance can be sought from the appropriate trade association

Description of manufacturing process

- ✓ In addition to chemical composition UVCB substances require information on source/manufacture
- ✓ To be provided in the description field of section 1.1 / section 3.1, or as an attachment in section 1.4
- ✓ Forms part of the substance identity - any significant change may lead to a different substance identity
- ✓ Should be provided in as much detail as possible
  - ✓ identity of starting materials/source (and ratio)
  - ✓ reaction steps/mechanisms
  - ✓ plant operating parameters (e.g. temperatures/pressures)
  - ✓ solvents/reagents used
  - ✓ details of any clean-up/purification steps
- ✓ Should be specific to the registered substance
- ⃠ Avoid a cut and paste of an EINECS description

Example of a description of a manufacturing process

1. An aqueous solution (...%) of A is acidified by addition of acid X in a 1:1 molar ratio to form B.
2. This solution is then reacted with C, which is dissolved in solvent Y, in a 1:2 molar ratio.
3. This 2-phase reaction forms the substance D, dissolved in solvent Y.
4. The aqueous layer is separated and disposed of.
5. The substance D is purified by distillation.

Constituents of UVCB substances

- ✓ Individual constituents > 10 % (w/w) or relevant for C&L and/or PBT assessment need to be specifically identified
- ✓ Constituents < 10 % (w/w) which have been specifically identified should be reported separately or as part of generic constituent
- ✓ Constituents which cannot be specifically identified or are to an extent unknown should be identified as far as possible and reported in generic terms
- ✓ It is important that close to 100 % accountability of the substance composition is achieved

Example of how to present generic constituents and concentration ranges

- A hydrocarbon-based UVCB substance has been analysed and contains > 50 constituents of which none are > 10 % in the chromatogram. The company has generically presented the composition as follows:
  - Linear alkanes (C20-C32) 60-80 % w/w
  - Branched alkanes (C20-C25) 20-35 w/w
  - Cyclic alkanes (C20-C25) 0-5 % w/w

Concentration ranges for constituents

- ✓ Always specify: for each specific and generic constituent listed in section 1.2
  - ✓ Minimum and maximum value (with units)
- ✓ Realistic: based on knowledge of production batches
  - ✓ They should not be overly broad
- ✓ Variability is an element of the definition of UVCB substance
- ✓ It assists ECHA in performing its tasks under REACH such as data sharing

Spectral data and analytical information fro UVCB substances

- Establishes the presence and absence of certain groups of constituents
- Registrants should not limit themselves to the basic set of techniques listed in Annex VI 2.3.5 and 2.3.6
- Where more information can be provided by techniques not listed in Annex VI section 2, this information should be included

Waiving of spectral data and analytical information

- **If it is not technically possible or if it does not appear scientifically necessary** to give information on one or more of the items listed in Annex VI, the **reasons shall be clearly stated** (Annex VI, Section 2)

🚫 The fact the substance is a UVCB is not a justification for waiving

✓ Important that these reasons are robust in their nature AND presented as scientifically-based justifications

✓ A more comprehensive analysis has been gained by using an alternative technique to those listed in Annex VI, Section 2

✓ However, it is still important that where the listed techniques are not applied the reason is explained

✓ Any justification for waiving will be assessed for its validity and consequently may not be accepted as valid

Example of a justification for waiving of spectral data

- A company produces a crystalline inorganic UVCB substance.
- The company considers that the list of spectral data in Annex VI 2.3.5 is not the best way to identify the substance but instead applies elemental analysis (XRF) as well as XRD and IR spectral analyses.
- These analyses characterise the substance.
- In addition the company waives NMR and UV spectral analysis based on the substance structure and the fact that more appropriate techniques have been applied instead.

Key messages for substance identity

- Information in the dossier should be sufficient to allow ECHA to conclude on an **unambiguous** substance identity
- All information should be **clear, concise and non-contradictory**
- Supplementary information can be attached in section 1.4
- ECHA does not have the same objectives with the use of spectral data and analytical information
- ECHA does not possess factual knowledge typically available to industry
- Support:
  - The inquiry TCC tool can be applied to your dossier
  - DSM Part 18 and the ECHA SID Guidance should be used to assist in the preparation of your registration dossier.

Thank You!

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